LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

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-BG090924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062866.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.770	112	116	124	rBV	43137	71890	5.59%	0.521%
2	4.363	213	217	222	rVB2	8238	11514	0.90%	0.083%
3	5.015	324	328	334	rVB2	8637	13070	1.02%	0.095%
4	5.251	363	368	374	rBV4	2679	4739	0.37%	0.034%
5	6.902	643	649	651	rBV5	1845	3628	0.28%	0.026%
6	7.072	669	678	685	rBV	103963	191007	14.86%	1.384%
7	7.231	698	705	713	rBV	63120	102126	7.94%	0.740%
8	7.330	717	722	728	rVB	20414	30248	2.35%	0.219%
9	7.436	733	740	748	rVB	93892	157737	12.27%	1.143%
10	7.548	756	759	764	rVB2	6098	8518	0.66%	0.062%
11	7.748	787	793	798	rBV2	6073	9444	0.73%	0.068%
12	7.900	809	819	827	rBV	150603	247112	19.22%	1.790%
13	8.018	834	839	842	rBV3	1793	3568	0.28%	0.026%
14	8.323	885	891	897	rBV	214840	340873	26.51%	2.469%
15	8.370	897	899	905	rVB3	7038	9446	0.73%	0.068%
16	8.517	918	924	932	rBV5	20553	33946	2.64%	0.246%
17	8.605	932	939	947	rVV	148580	253333	19.70%	1.835%
18	8.694	948	954	960	rVB6	5267	12578	0.98%	0.091%
19	8.887	983	987	996	rVB3	15637	25347	1.97%	0.184%
20	9.011	1003	1008	1010	rBV3	10064	16476	1.28%	0.119%
21	9.052	1010	1015	1023	rVV	96897	165270	12.85%	1.197%
22	9.234	1040	1046	1052	rVB2	2558	4837	0.38%	0.035%
23	9.475	1083	1087	1093	rVB4	3178	5391	0.42%	0.039%
24	9.616	1106	1111	1120	rVB4	13192	22640	1.76%	0.164%
25	9.775	1130	1138	1145	rBV4	88184	174491	13.57%	1.264%
26	10.121	1194	1197	1203	rVB3	2073	3900	0.30%	0.028%
27	10.192	1203	1209	1211	rBV4	2292	3911	0.30%	0.028%
28	10.227	1211	1215	1219	rVB5	4553	7784	0.61%	0.056%
29	10.315	1219	1230	1237	rBV	152321	284523	22.13%	2.061%
30	10.380	1237	1241	1247	rVB5	8403	13867	1.08%	0.100%
31	10.685	1282	1293	1301	rBV2	346351	649808	50.54%	4.707%
32	10.815	1308	1315	1329	rBV3	163357	407306	31.68%	2.950%
33	10.914	1329	1332	1337	rVV4	3591	5664	0.44%	0.041%
34	10.979	1338	1343	1346	rVV2	8052	12793	1.00%	0.093%
35	11.014	1346	1349	1353	rVB4	3776	5818	0.45%	0.042%
36	11.079	1356	1360	1366	rVB5	6647	11291	0.88%	0.082%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DDC50

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-BG090924.MA.M
Title : SVOA CALIBRATION

37	11.149	1368	1372	1376	rBV3	3269	4698	0.37%	0.034%
38	11.214	1376	1383	1388	rVB7	6434	14470	1.13%	0.105%
39	11.279	1388	1394	1398	rBV3	3641	5981	0.47%	0.043%
40	11.584	1437	1446	1451	rVV3	24123	40201	3.13%	0.291%
41	11.637	1451	1455	1459	rVB3	4696	6071	0.47%	0.044%
42	11.725	1465	1470	1476	rBV4	2930	5335	0.41%	0.039%
43	11.931	1499	1505	1510	rBV2	22413	34611	2.69%	0.251%
44	11.984	1510	1514	1520	rVB3	6527	10027	0.78%	0.073%
45	12.101	1529	1534	1540	rVB3	22863	35311	2.75%	0.256%
46	12.231	1545	1556	1561	rBV8	7824	22484	1.75%	0.163%
47	12.530	1604	1607	1612	rVB6	4468	7291	0.57%	0.053%
48	12.659	1626	1629	1633	rBV2	2923	3866	0.30%	0.028%
49	13.100	1696	1704	1710	rBV	36802	56525	4.40%	0.409%
50	13.171	1714	1716	1723	rVB4	2289	3856	0.30%	0.028%
51	13.353	1744	1747	1752	rBV3	3297	4803	0.37%	0.035%
52	13.500	1767	1772	1776	rVB4	3125	4511	0.35%	0.033%
53	13.582	1781	1786	1792	rBV2	2494	3640	0.28%	0.026%
54	13.746	1808	1814	1820	rVB3	4771	8653	0.67%	0.063%
55	13.823	1820	1827	1828	rBV4	4730	9316	0.72%	0.067%
56	13.934	1839	1846	1853	rVB	322661	474334	36.89%	3.436%
57	14.140	1879	1881	1886	rVV5	5222	7975	0.62%	0.058%
58	14.222	1888	1895	1902	rVB2	337423	532412	41.41%	3.857%
59	14.305	1905	1909	1912	rBV5	8001	10013	0.78%	0.073%
60	14.416	1924	1928	1934	rBV5	5929	9286	0.72%	0.067%
61	14.481	1934	1939	1941	rBV3	6515	10270	0.80%	0.074%
62	14.528	1941	1947	1954	rVB	436107	646055	50.25%	4.680%
63	14.728	1974	1981	1988	rBV2	130913	225120	17.51%	1.631%
64	14.869	2003	2005	2010	rVB5	4219	5006	0.39%	0.036%
65	14.933	2012	2016	2018	rBV3	2672	3553	0.28%	0.026%
66	15.063	2031	2038	2042	rBV5	4278	7294	0.57%	0.053%
67	15.104	2042	2045	2049	rVV3	4059	6176	0.48%	0.045%
68	15.151	2049	2053	2058	rVB6	4188	7173	0.56%	0.052%
69	15.380	2089	2092	2099	rVB4	3506	5702	0.44%	0.041%
70	15.521	2109	2116	2122	rBV	531496	760422	59.15%	5.508%
71	15.580	2124	2126	2130	rVV2	3449	4728	0.37%	0.034%
72	15.638	2130	2136	2142	rVV	136962	197666	15.37%	1.432%
73	15.697	2142	2146	2152	rVB5	4388	7366	0.57%	0.053%
74	15.762	2152	2157	2160	rBV4	5279	7834	0.61%	0.057%
75	15.885	2171	2178	2183	rBV	44461	66512	5.17%	0.482%
76	16.238	2233	2238	2242	rBV4	3459	4939	0.38%	0.036%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

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-BG090924.MA.M
Title : SVOA CALIBRATION

77	16.578	2292	2296	2300	rBV3	2510	3207	0.25%	0.023%
78	16.672	2306	2312	2314	rBV	2937	4339	0.34%	0.031%
79	16.925	2350	2355	2362	rBV2	14575	23379	1.82%	0.169%
80	17.037	2369	2374	2375	rBV2	3324	3593	0.28%	0.026%
81	17.272	2408	2414	2422	rBV	636801	916234	71.26%	6.637%
82	17.372	2424	2431	2438	rVB	637365	930934	72.41%	6.743%
83	17.454	2444	2445	2449	rVB3	4952	5115	0.40%	0.037%
84	17.771	2493	2499	2502	rBV3	3946	5858	0.46%	0.042%
85	17.889	2515	2519	2524	rBV4	14440	21158	1.65%	0.153%
86	18.165	2561	2566	2576	rBV	90694	142564	11.09%	1.033%
87	18.464	2613	2617	2622	rBV7	4136	7246	0.56%	0.052%
88	19.228	2743	2747	2751	rBV3	10100	14820	1.15%	0.107%
89	19.299	2755	2759	2761	rBV	12631	17060	1.33%	0.124%
90	19.440	2780	2783	2788	rBV4	11988	16271	1.27%	0.118%
91	19.593	2807	2809	2813	rVB4	6598	6656	0.52%	0.048%
92	19.663	2815	2821	2826	rBV	853013	1196863	93.09%	8.670%
93	19.704	2826	2828	2831	rVB3	11442	11279	0.88%	0.082%
94	20.168	2905	2907	2910	rBV4	4889	5649	0.44%	0.041%
95	20.204	2910	2913	2916	rVB5	7091	8289	0.64%	0.060%
96	21.185	3075	3080	3086	rBV2	89434	132605	10.31%	0.961%
97	21.520	3130	3137	3148	rBV	748488	1156963	89.99%	8.381%
98	21.714	3167	3170	3174	rBV3	9896	12194	0.95%	0.088%
99	24.369	3613	3622	3635	rVB	483350	1285689	100.00%	9.313%
100	24.581	3648	3658	3671	rVB	469753	1270042	98.78%	9.200%

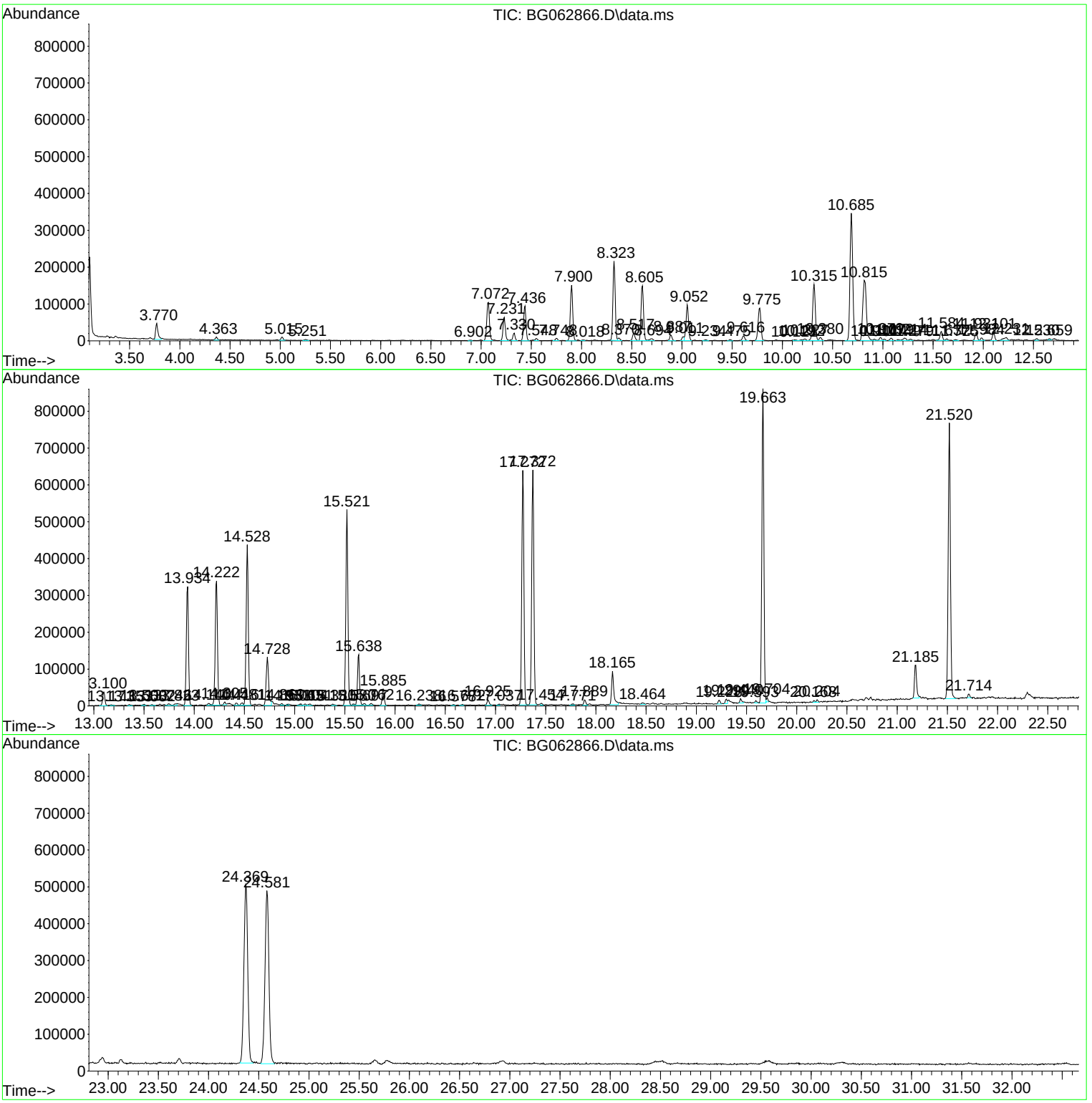
Sum of corrected areas: 13805387

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.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\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

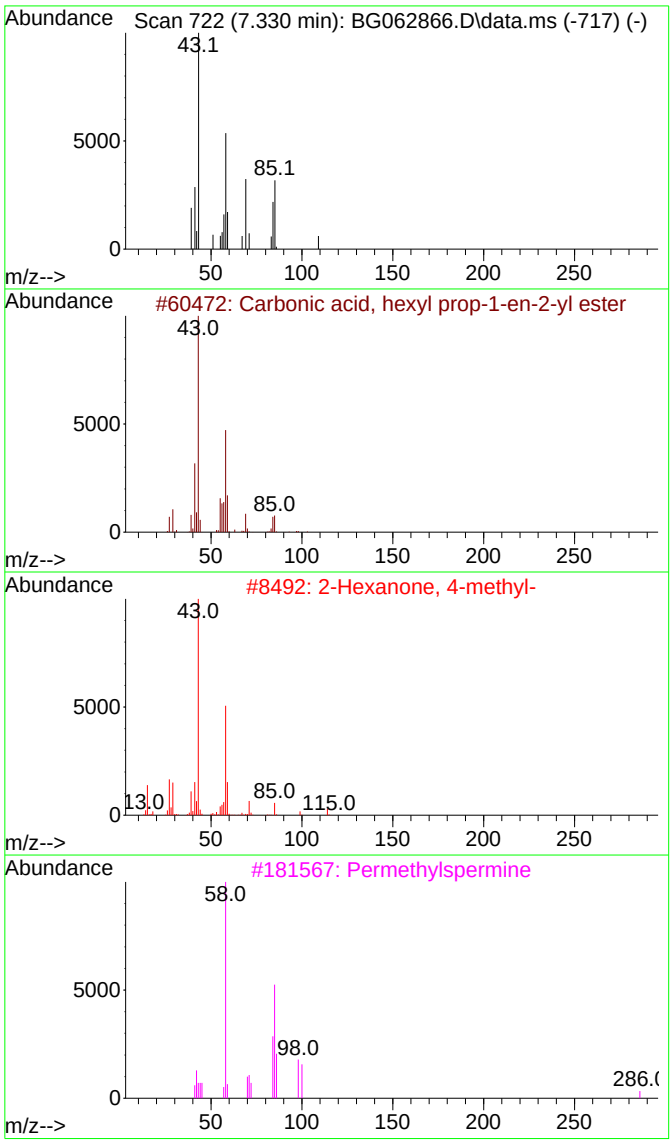
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

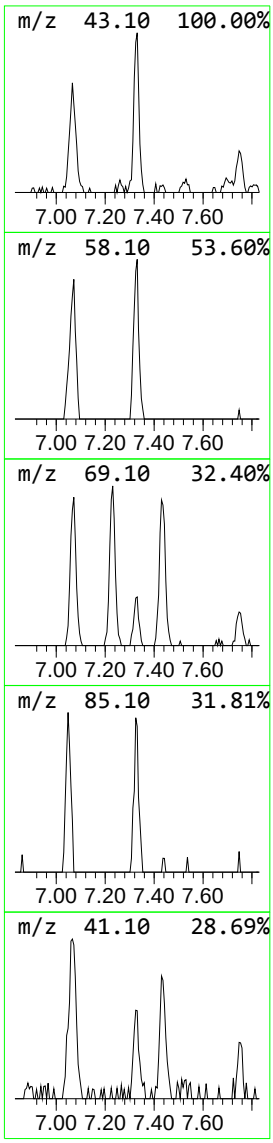
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Carbonic acid, hexyl prop-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.330	2.45 ng/ul	30248	1,4-Dichlorobenzene-d4	7.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	64
2	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	47
3	Permethylspermine	286	C16H38N4	057905-96-1	42
4	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	39
5	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

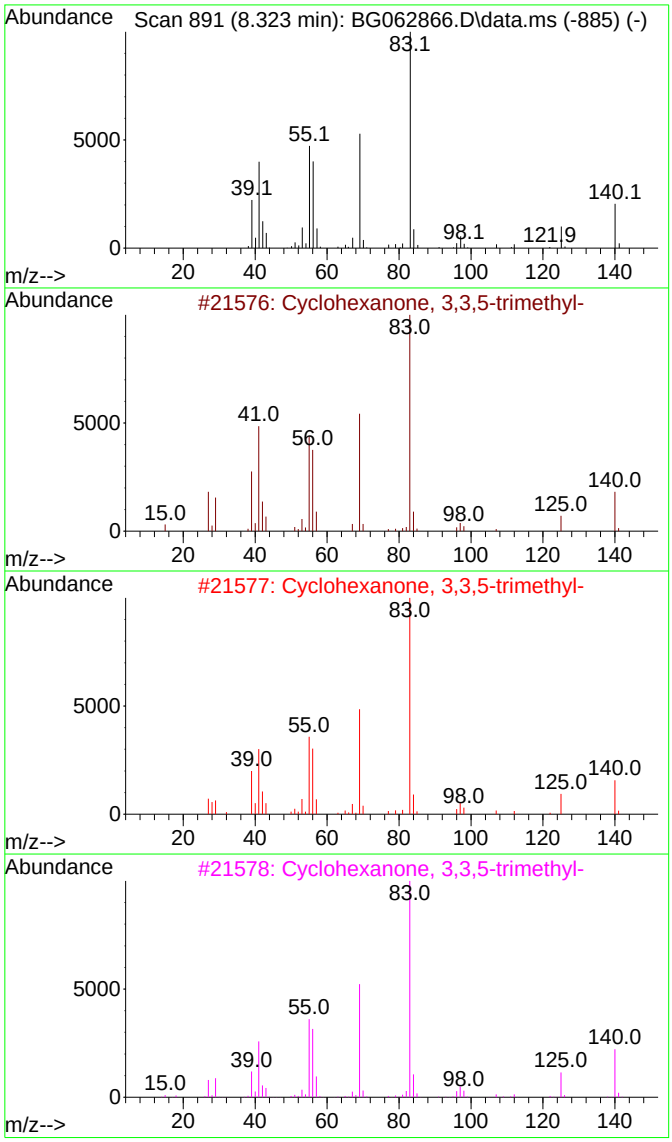
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

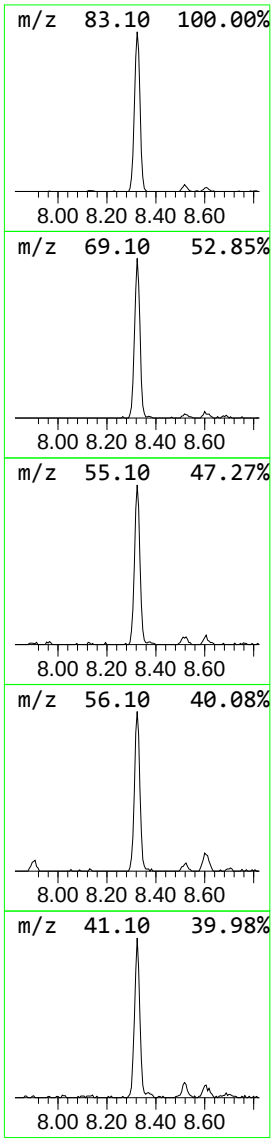
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.323	27.59 ng/ul	340873	1,4-Dichlorobenzene-d4	7.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
2	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
3	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	94
4	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	87
5	Cyclopentanone, 3-butyl-	140	C9H16O	057283-81-5	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

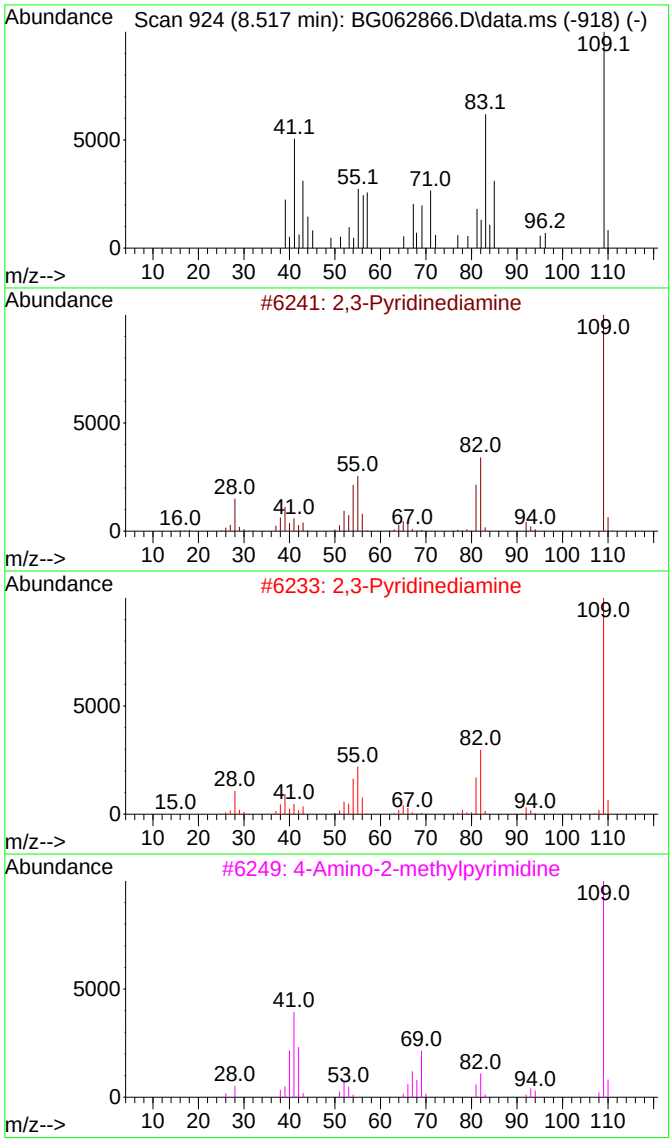
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

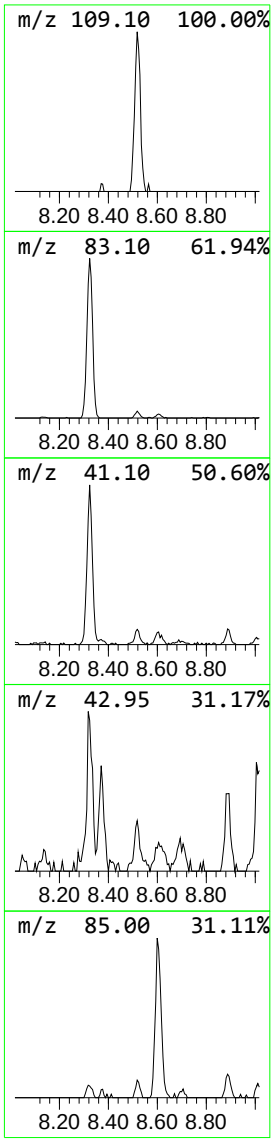
****

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.517	2.75 ng/ul	33946	1,4-Dichlorobenzene-d4	7.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Pyridinediamine	109	C5H7N3	000452-58-4	27
2	2,3-Pyridinediamine	109	C5H7N3	000452-58-4	27
3	4-Amino-2-methylpyrimidine	109	C5H7N3	000074-69-1	27
4	3,4-Pyridinediamine	109	C5H7N3	000054-96-6	27
5	2-Amino-4-methylpyrimidine	109	C5H7N3	000108-52-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

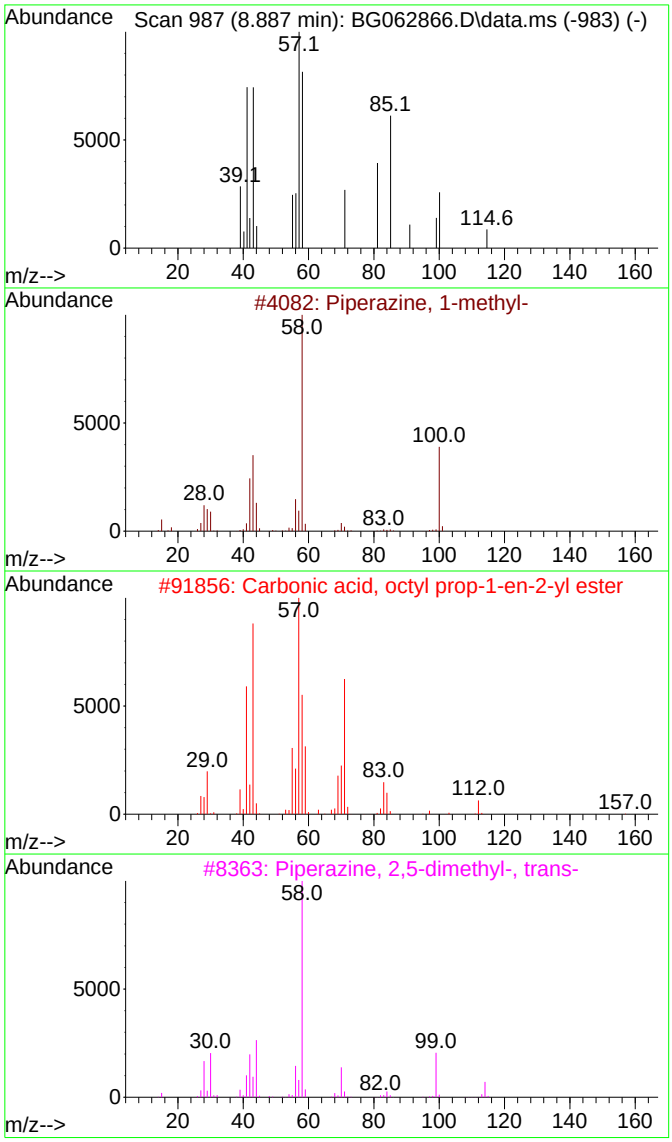
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

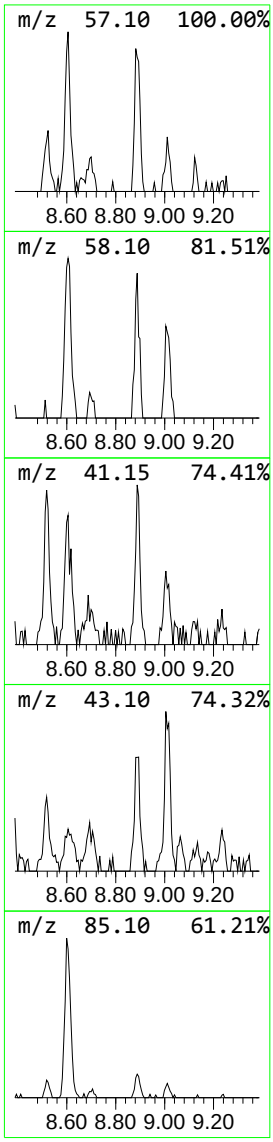
****

Peak Number 4 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.887	2.05 ng/ul	25347	1,4-Dichlorobenzene-d4	7.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperazine, 1-methyl-	100	C5H12N2	000109-01-3	32
2	Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	23
3	Piperazine, 2,5-dimethyl-, trans-	114	C6H14N2	002815-34-1	17
4	3-Methyl-3-hexen-2-ol	114	C7H14O	076966-27-3	14
5	Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

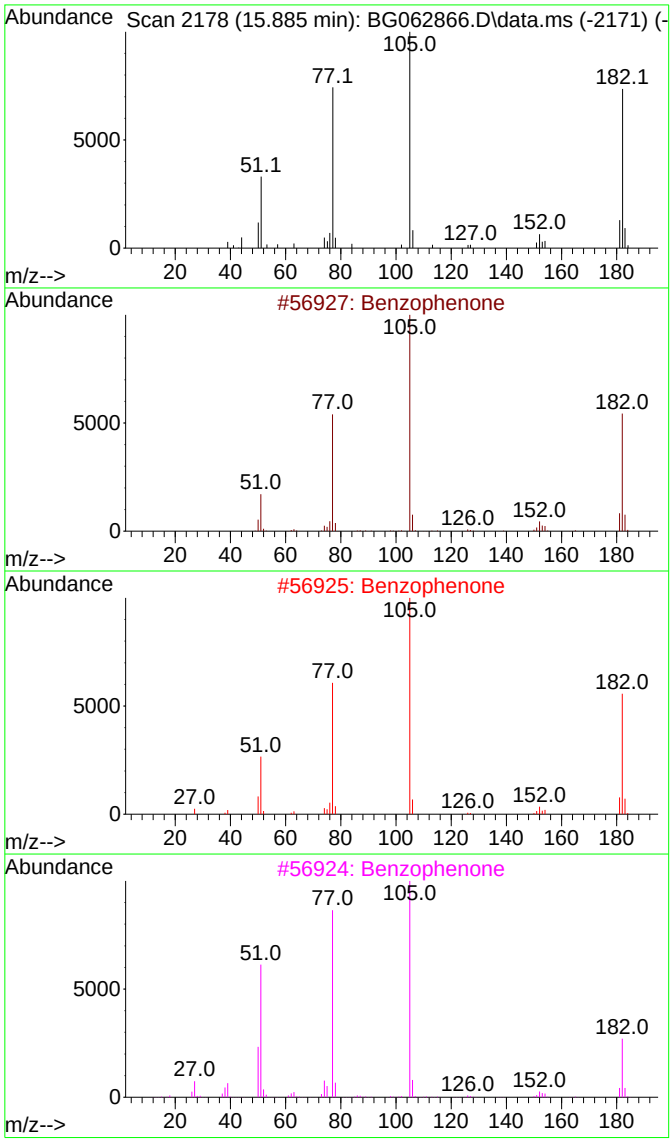
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

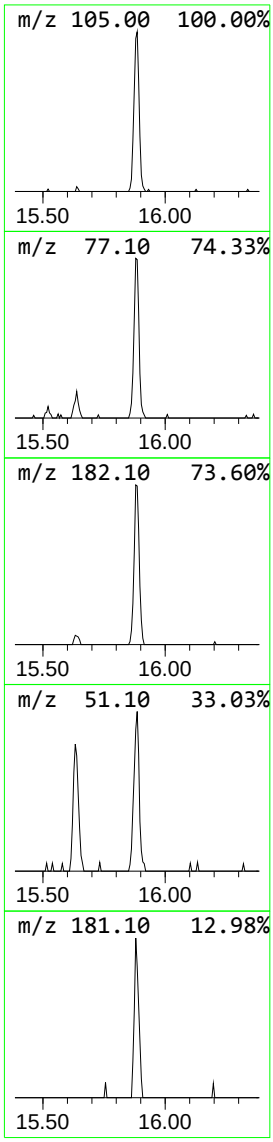
****

Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.885	2.06 ng/ul	66512	Acenaphthene-d10	14.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	94
5	Benzophenone	182	C13H10O	000119-61-9	91





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Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

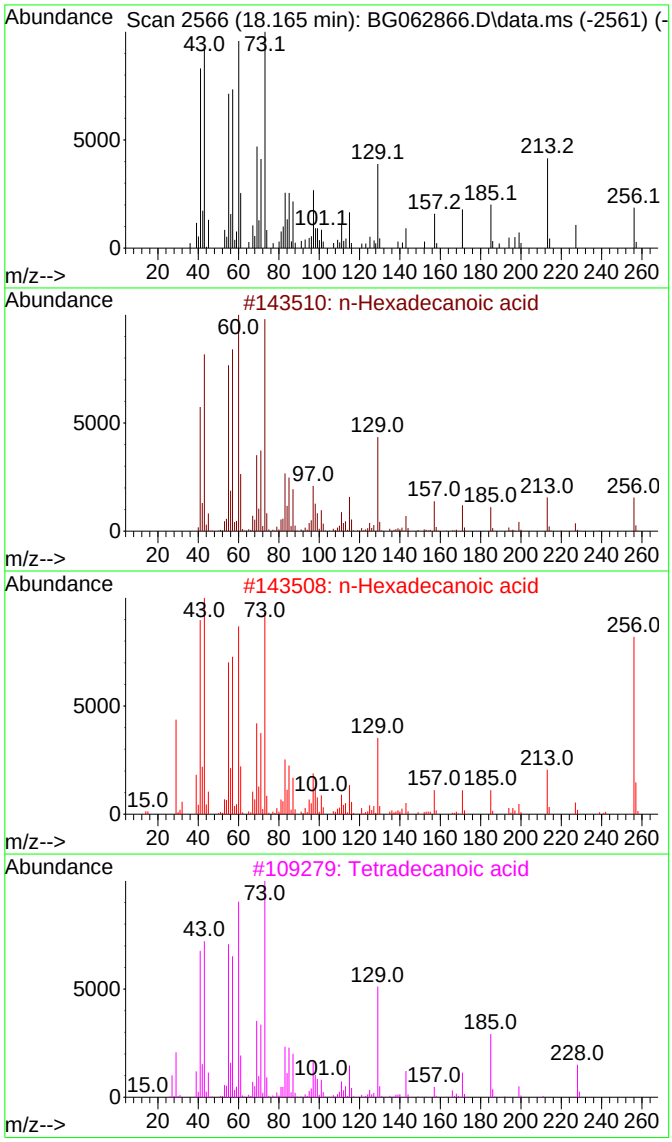
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

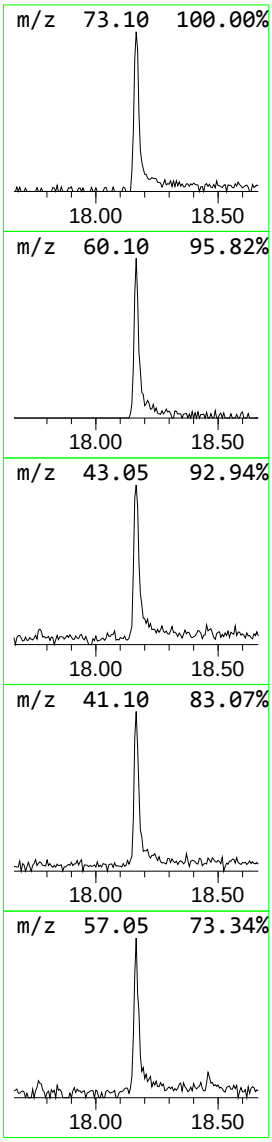
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.165	3.11 ng/ul	142564	Phenanthrene-d10	17.272

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

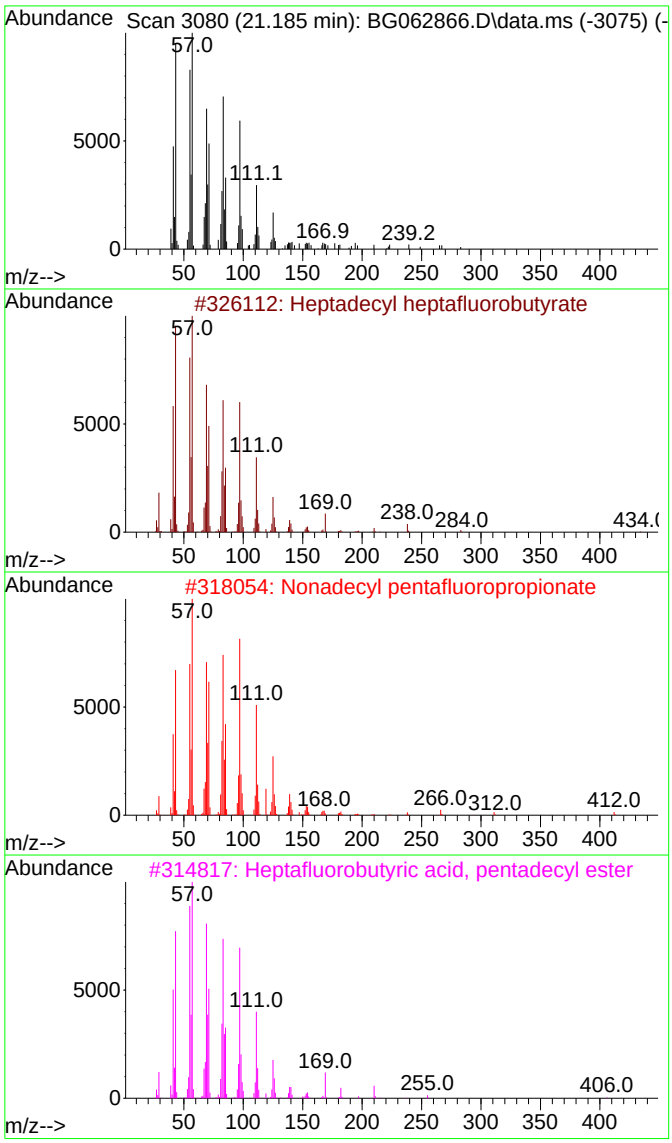
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.MA.M
Quant Title : SVOA CALIBRATION

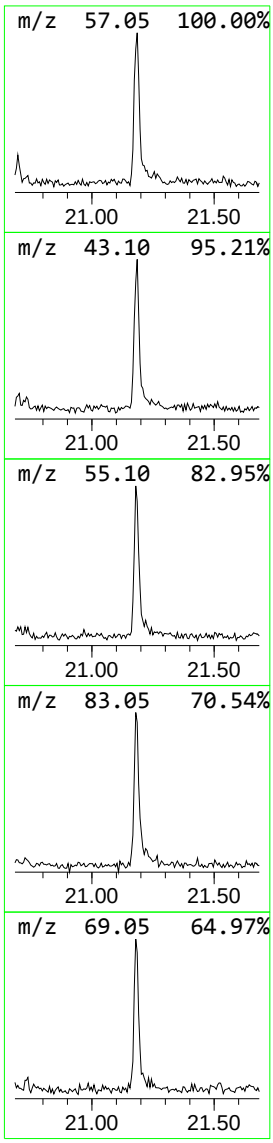
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.185	2.29 ng/ul	132605	Chrysene-d12	21.520

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091324\
Data File : BG062866.D
Acq On : 16 Sep 2024 4:38
Operator : JU/RC
Sample : P3899-14
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC50

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG090924.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
Carbonic acid, ...	7.330	2.5	ng/ul	30248	1	7.900	247112	20.0
Cyclohexanone, ...	8.323	27.6	ng/ul	340873	1	7.900	247112	20.0
unknown-01	8.517	2.8	ng/ul	33946	1	7.900	247112	20.0
unknown-02	8.887	2.0	ng/ul	25347	1	7.900	247112	20.0
Benzophenone	15.885	2.1	ng/ul	66512	3	14.528	646055	20.0
n-Hexadecanoic ...	18.165	3.1	ng/ul	142564	4	17.272	916234	20.0
Heptadecyl hept...	21.185	2.3	ng/ul	132605	5	21.520	1156960	20.0