LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

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-BG112024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG063539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.217	19	22	25	rBV4	11490	15083	0.40%	0.037%
2	3.300	32	36	39	rVB3	19078	23388	0.61%	0.058%
3	4.034	158	161	165	rBV5	7630	11186	0.29%	0.028%
4	4.956	316	318	321	rVB3	6970	6307	0.17%	0.016%
5	5.121	343	346	350	rBV3	6039	10294	0.27%	0.025%
6	5.297	373	376	380	rVB4	4958	7819	0.20%	0.019%
7	6.519	578	584	589	rBV4	16101	29393	0.77%	0.073%
8	6.784	625	629	633	rVB4	9500	13844	0.36%	0.034%
9	7.007	658	667	684	rBV	360304	673761	17.65%	1.663%
10	7.160	687	693	701	rVV	268783	427054	11.18%	1.054%
11	7.271	706	712	716	rBV5	22174	35869	0.94%	0.089%
12	7.365	722	728	735	rBV	345212	581384	15.23%	1.435%
13	7.730	785	790	797	rVB3	27668	45201	1.18%	0.112%
14	7.830	800	807	814	rVV	441489	732163	19.18%	1.807%
15	7.894	815	818	823	rVB6	5781	8457	0.22%	0.021%
16	8.047	840	844	853	rBV6	8759	16256	0.43%	0.040%
17	8.540	922	928	935	rBV	469841	801192	20.98%	1.978%
18	8.587	935	936	940	rVB3	9001	7220	0.19%	0.018%
19	8.981	996	1003	1015	rBV	344299	623335	16.33%	1.539%
20	9.146	1027	1031	1032	rBV2	5168	6069	0.16%	0.015%
21	9.404	1072	1075	1080	rVB3	9017	15574	0.41%	0.038%
22	9.545	1095	1099	1108	rBV5	23948	40670	1.07%	0.100%
23	9.704	1120	1126	1136	rBV	311000	573539	15.02%	1.416%
24	10.250	1210	1219	1229	rBV2	462032	862166	22.58%	2.128%
25	10.620	1274	1282	1289	rBV	608358	1101402	28.85%	2.719%
26	10.756	1297	1305	1318	rBV2	255427	520627	13.64%	1.285%
27	10.949	1336	1338	1342	rVB2	4591	7429	0.19%	0.018%
28	11.014	1347	1349	1352	rBV3	5291	6417	0.17%	0.016%
29	11.161	1370	1374	1376	rBV4	13190	16886	0.44%	0.042%
30	11.261	1387	1391	1395	rBV3	6043	6670	0.17%	0.016%
31	11.778	1476	1479	1484	rVB6	4194	7005	0.18%	0.017%
32	12.042	1521	1524	1527	rVB3	6029	6753	0.18%	0.017%
33	12.113	1533	1536	1537	rBV	6376	5979	0.16%	0.015%
34	12.207	1549	1552	1554	rBV3	6623	7574	0.20%	0.019%
35	12.677	1628	1632	1637	rVB2	5229	8272	0.22%	0.020%
36	12.835	1651	1659	1667	rBV7	29143	61955	1.62%	0.153%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
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Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

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-BG112024.MA.M
Title : SVOA CALIBRATION

37	12.924	1671	1674	1678	rBV4	8846	11880	0.31%	0.029%
38	13.070	1697	1699	1704	rVB4	5692	6315	0.17%	0.016%
39	13.206	1717	1722	1731	rBV9	40940	82712	2.17%	0.204%
40	13.300	1736	1738	1742	rVV5	6673	9735	0.25%	0.024%
41	13.347	1742	1746	1751	rVB4	50056	80478	2.11%	0.199%
42	13.740	1808	1813	1817	rBV5	16347	23557	0.62%	0.058%
43	13.799	1819	1823	1830	rVB7	14284	23933	0.63%	0.059%
44	13.875	1830	1836	1845	rBV	955891	1394820	36.53%	3.443%
45	14.075	1867	1870	1872	rBV4	8900	11939	0.31%	0.029%
46	14.122	1874	1878	1879	rVV4	8074	8015	0.21%	0.020%
47	14.163	1879	1885	1893	rVB	1022486	1612546	42.23%	3.981%
48	14.310	1906	1910	1915	rBV3	55902	76132	1.99%	0.188%
49	14.434	1925	1931	1933	rBV2	297238	422102	11.05%	1.042%
50	14.469	1933	1937	1945	rVB	1040269	1580862	41.40%	3.902%
51	14.545	1946	1950	1954	rVB3	55962	66874	1.75%	0.165%
52	14.592	1956	1958	1962	rVB3	17100	20695	0.54%	0.051%
53	14.686	1965	1974	1979	rBV	304696	568046	14.88%	1.402%
54	14.798	1988	1993	1998	rVB3	56670	100090	2.62%	0.247%
55	14.898	2005	2010	2015	rBV7	19160	28548	0.75%	0.070%
56	15.003	2024	2028	2033	rBV5	15709	19749	0.52%	0.049%
57	15.080	2039	2041	2046	rVB3	6983	10468	0.27%	0.026%
58	15.139	2046	2051	2053	rBV3	8023	13370	0.35%	0.033%
59	15.280	2074	2075	2078	rVB3	8002	6153	0.16%	0.015%
60	15.333	2081	2084	2085	rVV2	8528	8156	0.21%	0.020%
61	15.356	2085	2088	2092	rVB5	21575	31030	0.81%	0.077%
62	15.468	2098	2107	2113	rBV	1404173	2074952	54.34%	5.122%
63	15.597	2123	2129	2138	rBV	358828	581032	15.22%	1.434%
64	15.703	2145	2147	2154	rVB8	14121	21786	0.57%	0.054%
65	15.832	2161	2169	2177	rBV	510305	763012	19.98%	1.883%
66	15.949	2184	2189	2193	rVB6	55742	97899	2.56%	0.242%
67	16.043	2200	2205	2210	rBV8	30926	53845	1.41%	0.133%
68	16.126	2214	2219	2222	rVB7	19196	29679	0.78%	0.073%
69	16.196	2227	2231	2235	rVV6	15724	19673	0.52%	0.049%
70	16.261	2237	2242	2249	rBV2	111146	144876	3.79%	0.358%
71	16.325	2249	2253	2256	rBV7	18275	25675	0.67%	0.063%
72	16.396	2261	2265	2270	rVB4	25537	38167	1.00%	0.094%
73	16.484	2278	2280	2283	rBV3	5525	6070	0.16%	0.015%
74	16.848	2338	2342	2343	rBV3	5004	6314	0.17%	0.016%
75	17.101	2382	2385	2387	rBV4	8587	9434	0.25%	0.023%
76	17.136	2389	2391	2395	rBV5	12959	17977	0.47%	0.044%

LSC Area Percent Report

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Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

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
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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Title : SVOA CALIBRATION

77	17.224	2399	2406	2414	rVV	1557111	2297808	60.18%	5.672%
78	17.324	2417	2423	2432	rVV	1639012	2384859	62.46%	5.887%
79	17.900	2516	2521	2523	rBV6	14004	19631	0.51%	0.048%
80	18.076	2549	2551	2554	rBV4	11571	7304	0.19%	0.018%
81	18.129	2555	2560	2569	rBV2	260599	474291	12.42%	1.171%
82	18.423	2606	2610	2615	rVB6	39631	63126	1.65%	0.156%
83	18.546	2629	2631	2632	rBV2	11252	7229	0.19%	0.018%
84	19.263	2750	2753	2754	rBV3	23601	27349	0.72%	0.068%
85	19.293	2754	2758	2771	rVV	360354	661664	17.33%	1.633%
86	19.622	2809	2814	2820	rBV	2059221	2950678	77.28%	7.284%
87	20.973	3039	3044	3051	rVB	2977862	3818229	100.00%	9.425%
88	21.149	3069	3074	3086	rBV	339223	571183	14.96%	1.410%
89	21.484	3125	3131	3140	rVB	1790096	2737839	71.70%	6.758%
90	22.271	3261	3265	3278	rVB4	155635	318580	8.34%	0.786%
91	23.652	3495	3500	3506	rVB	125783	235286	6.16%	0.581%
92	24.316	3603	3613	3625	rBV	1146459	3007251	78.76%	7.423%
93	24.528	3639	3649	3659	rBV	1205922	3106564	81.36%	7.668%
94	25.573	3823	3827	3839	rVB2	125881	340749	8.92%	0.841%
95	29.434	4480	4484	4485	rBV4	33943	48650	1.27%	0.120%

Sum of corrected areas: 40511059

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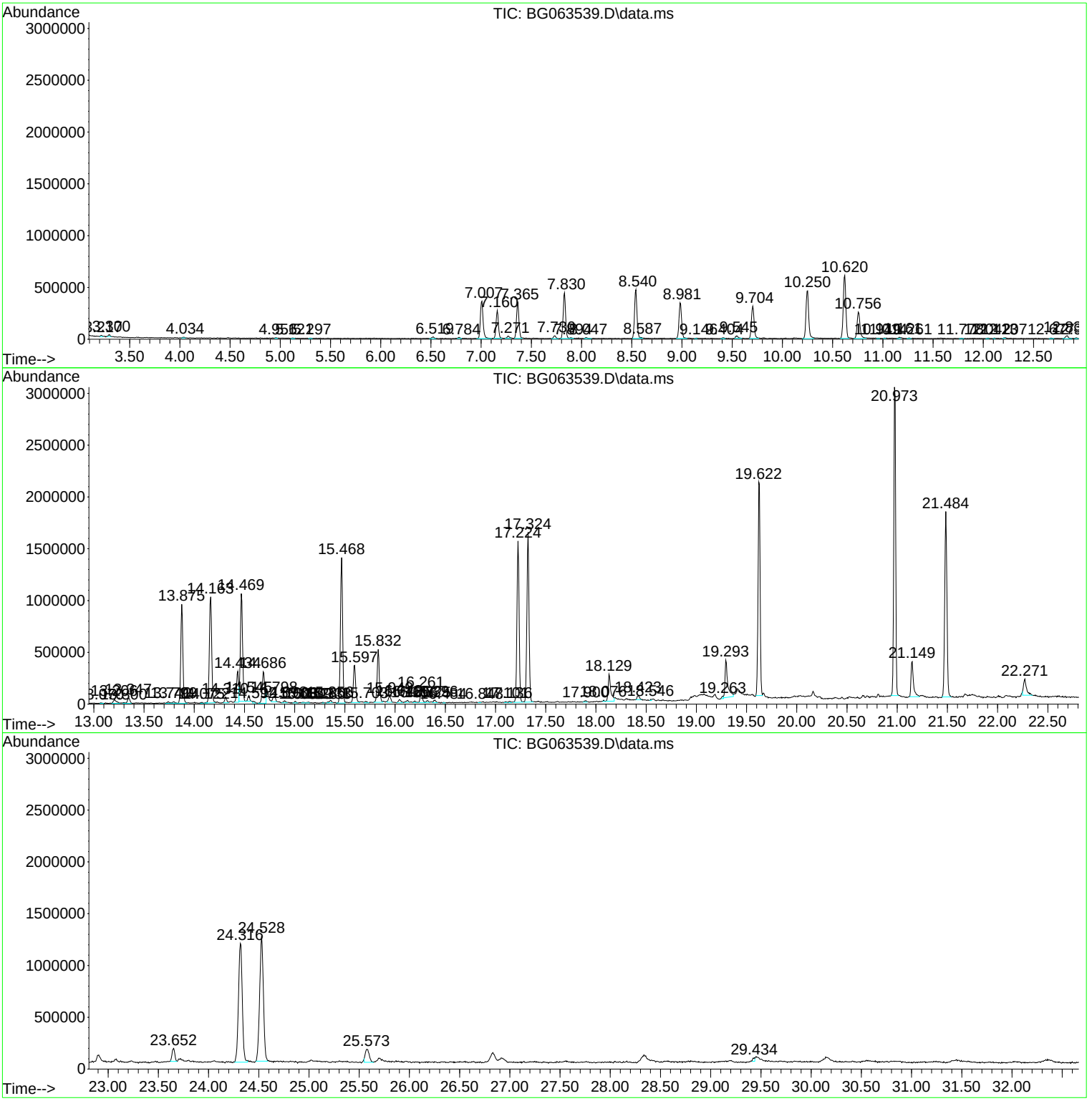
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.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\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
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Instrument :
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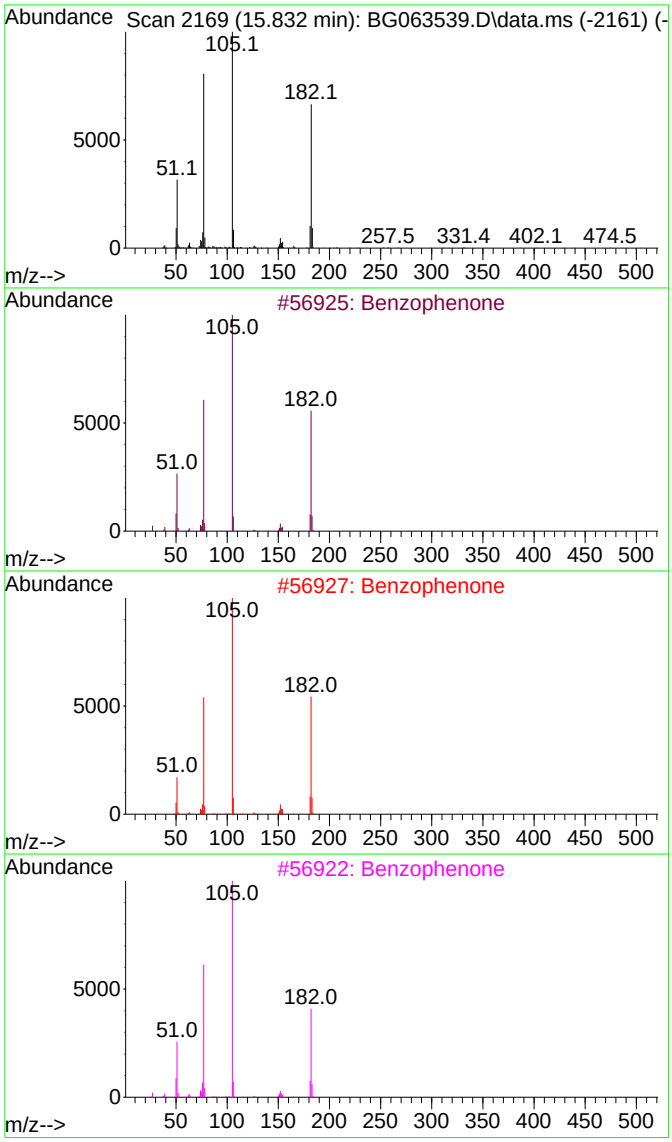
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

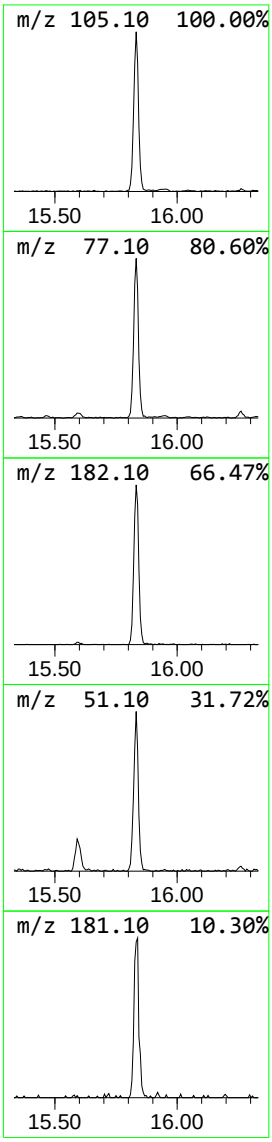
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.832	9.65 ng/ul	763012	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	91
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

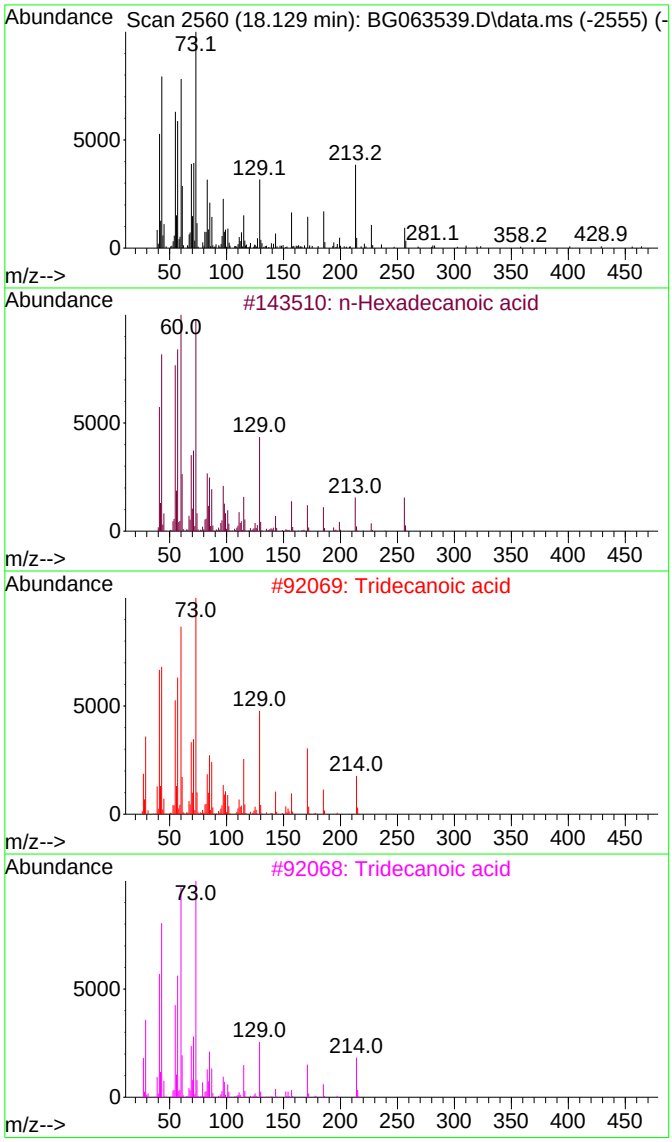
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

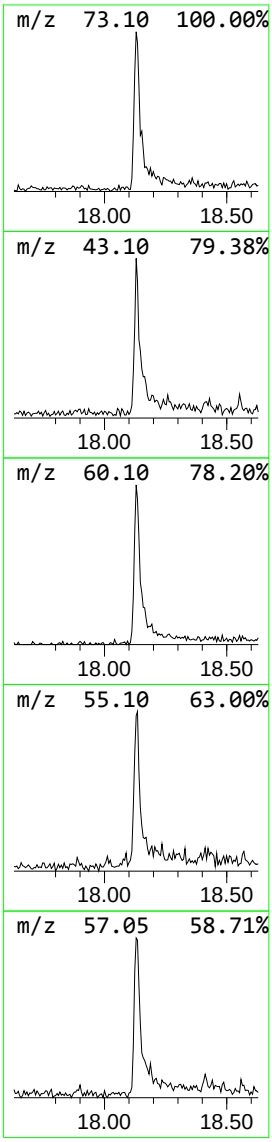
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.129	4.13 ng/ul	474291	Phenanthrene-d10	17.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

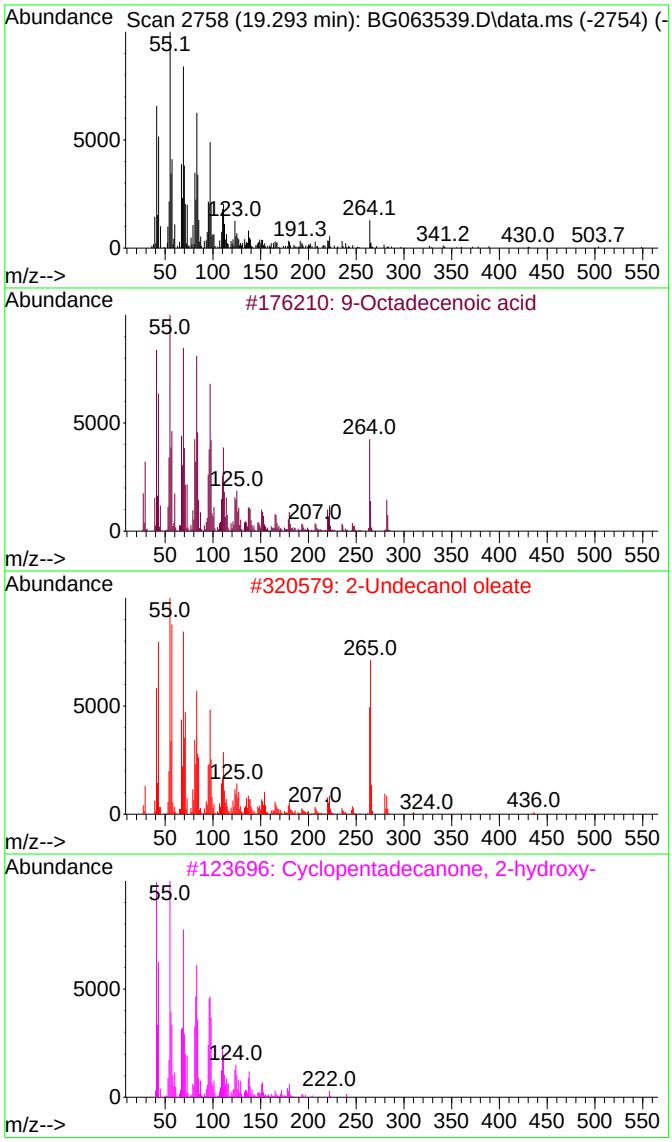
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

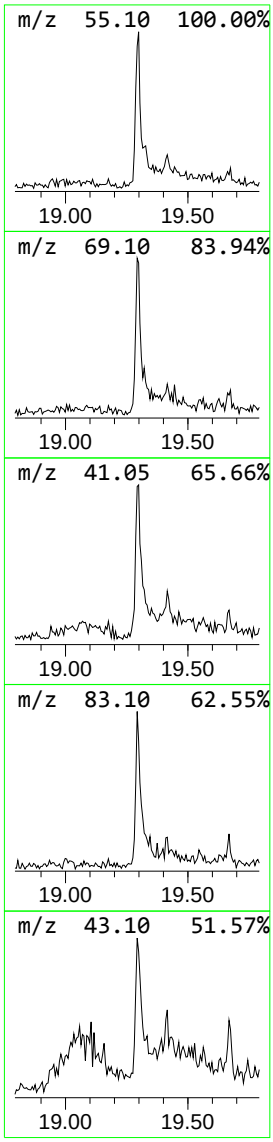
****

Peak Number 3 9-Octadecenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.293	5.76 ng/ul	661664	Phenanthrene-d10	17.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid	282	C18H34O2	002027-47-6	91
2	2-Undecanol oleate	436	C29H56O2	1000465-66-9	87
3	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	74
4	Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	53
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
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Acq On : 23 Nov 2024 3:52
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Sample : P4881-05
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ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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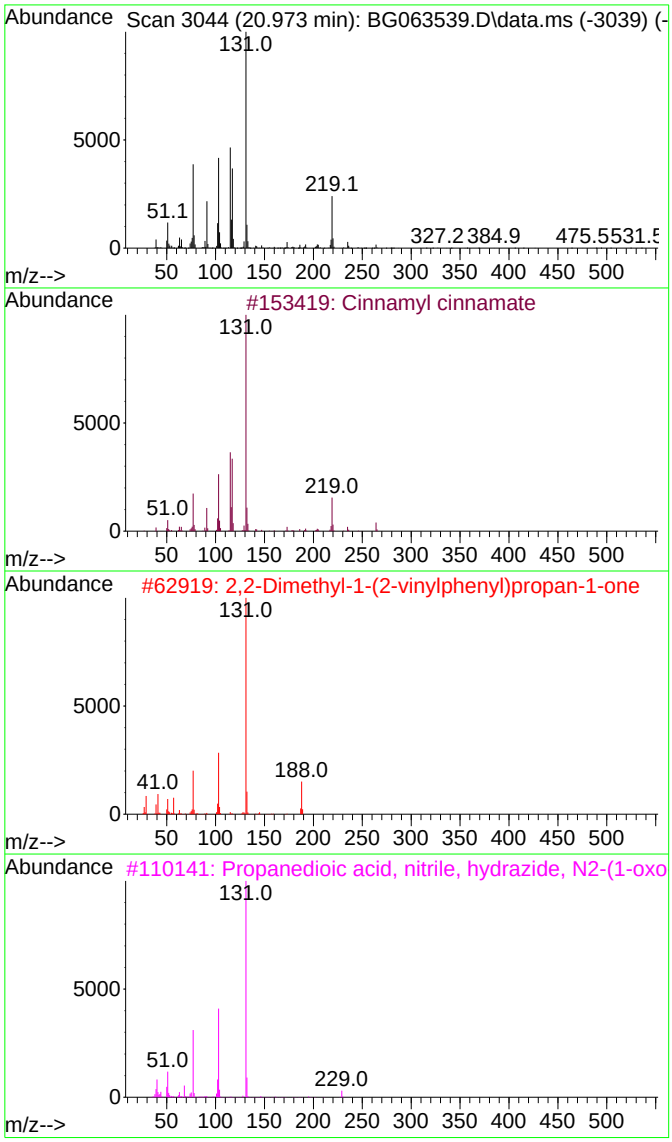
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

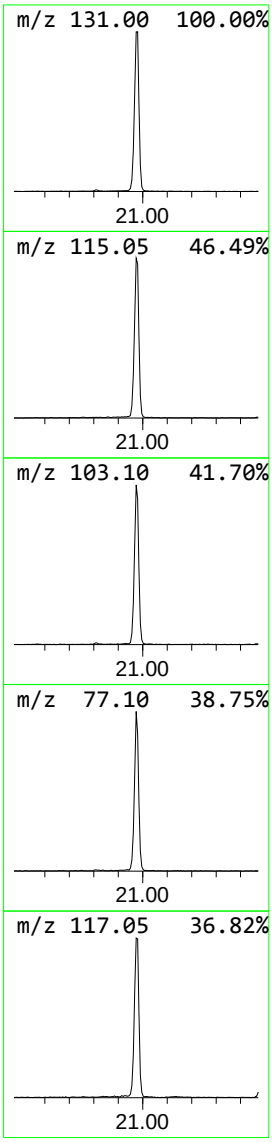
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	27.89 ng/ul	3818230	Chrysene-d12	21.484

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	50
4	3-Phenyl-N-m-tolyl-acrylamide	237	C16H15NO	1000296-12-9	50
5	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	50





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Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

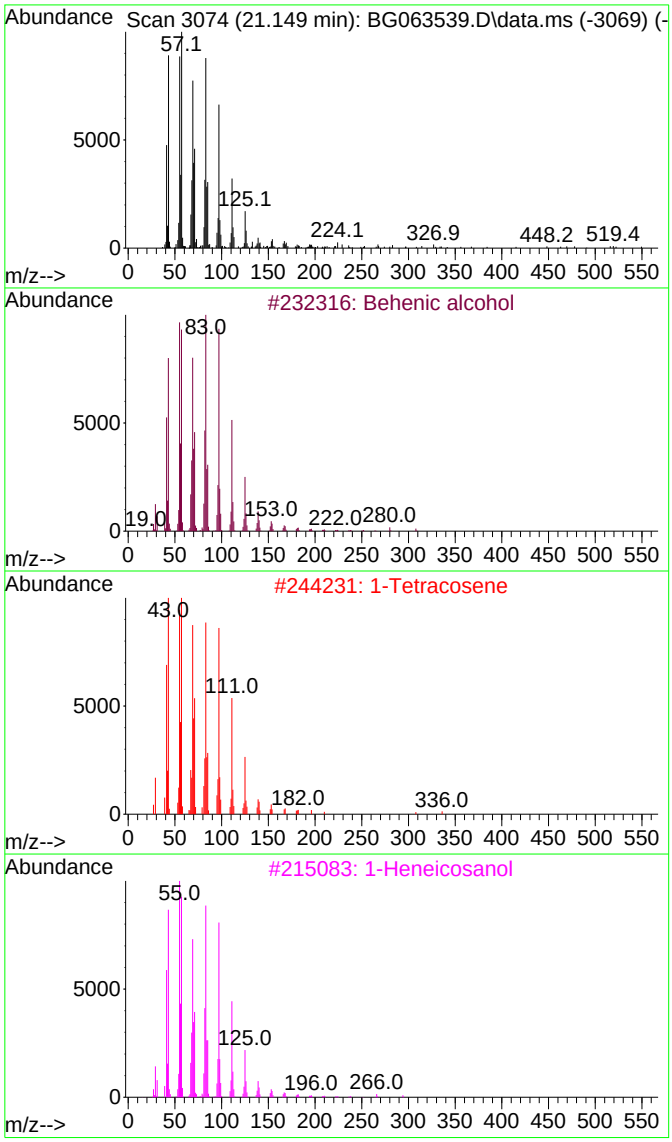
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

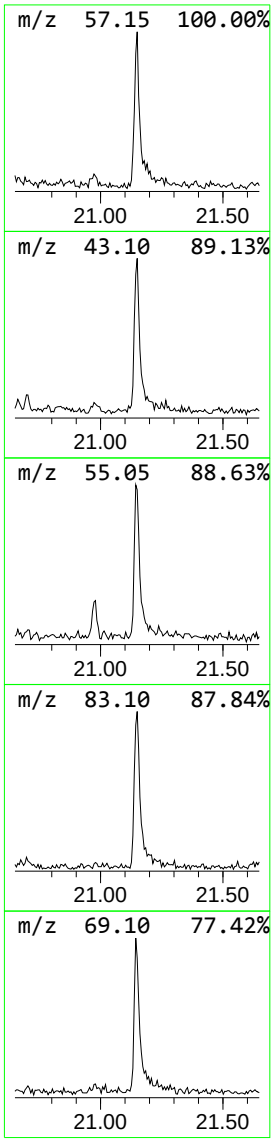
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.149	4.17 ng/ul	571183	Chrysene-d12	21.484

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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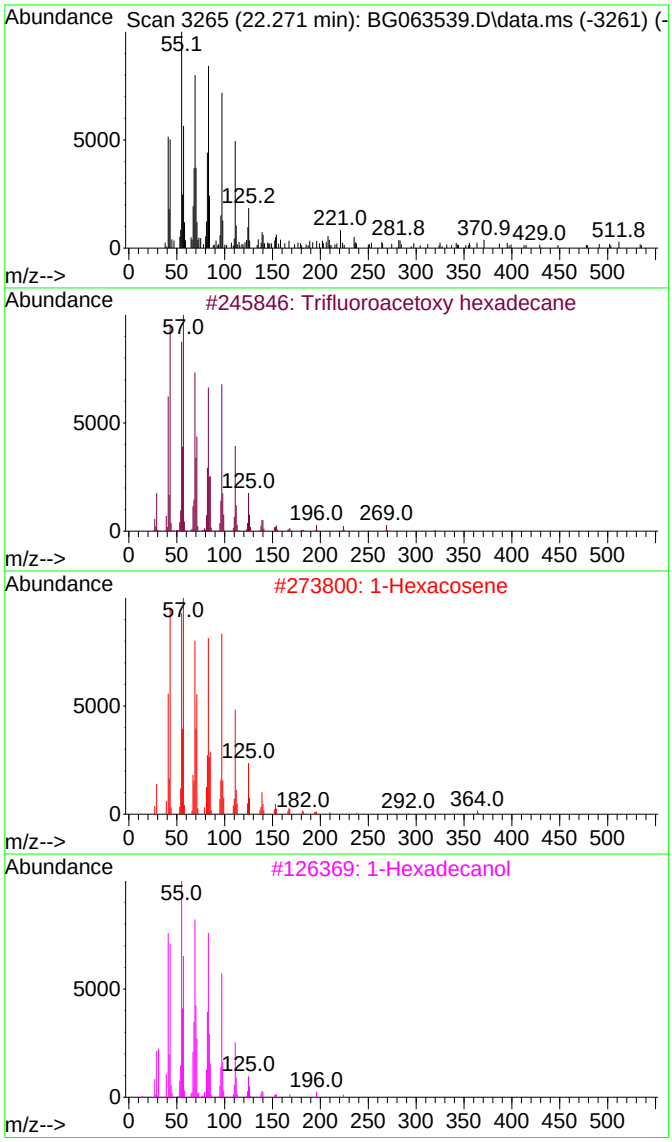
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

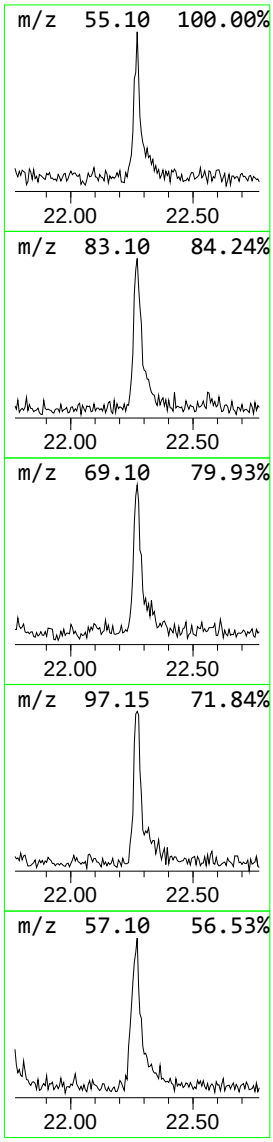
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.271	2.33 ng/ul	318580	Chrysene-d12	21.484

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2	1-Hexacosene	364	C26H52	018835-33-1	90
3	1-Hexadecanol	242	C16H34O	036653-82-4	80
4	1-Hexadecanol	242	C16H34O	036653-82-4	80
5	Oleic Acid	282	C18H34O2	000112-80-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

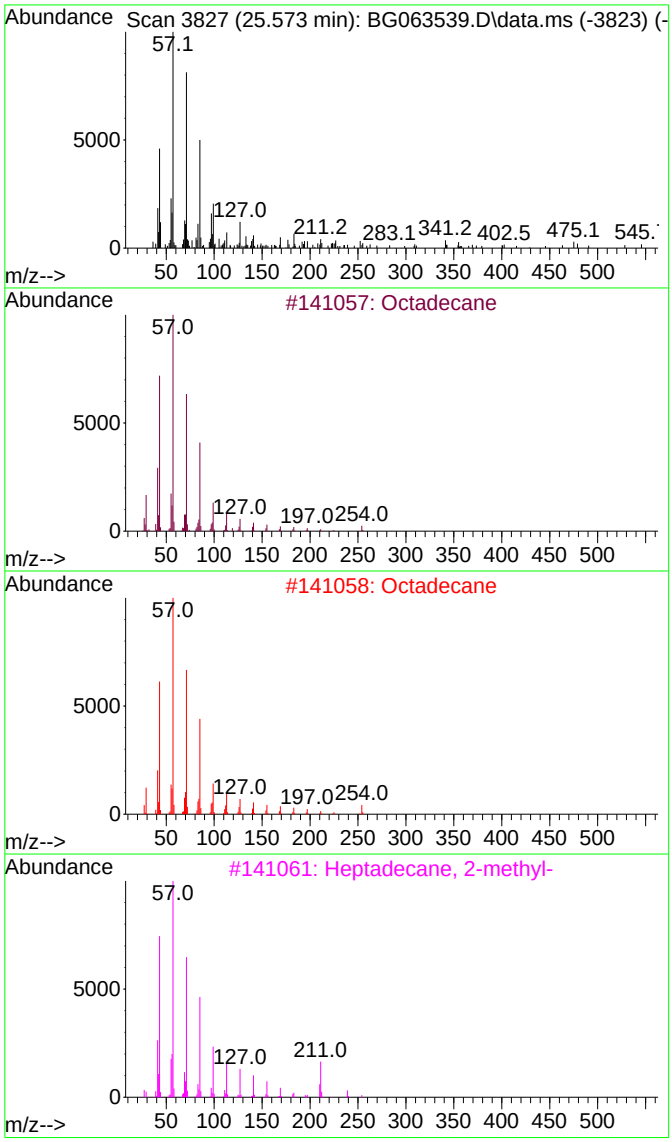
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.MA.M
Quant Title : SVOA CALIBRATION

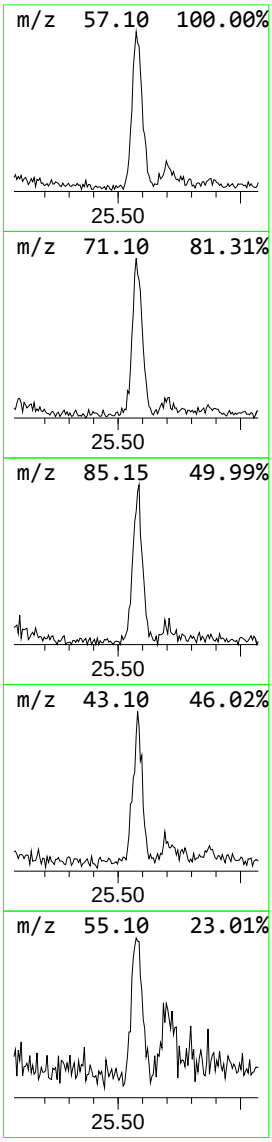
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.573	2.19 ng/ul	340749	Perylene-d12	24.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Octadecane	254	C18H38	000593-45-3	87
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112224\
Data File : BG063539.D
Acq On : 23 Nov 2024 3:52
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0TF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112024.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
Benzophenone	15.832	9.7	ng/ul	763012	3	14.469	1580860	20.0
n-Hexadecanoic ...	18.129	4.1	ng/ul	474291	4	17.224	2297810	20.0
9-Octadecenoic ...	19.293	5.8	ng/ul	661664	4	17.224	2297810	20.0
Cinnamyl cinnamate	20.973	27.9	ng/ul	3818230	5	21.484	2737840	20.0
Behenic alcohol	21.149	4.2	ng/ul	571183	5	21.484	2737840	20.0
Trifluoroacetox...	22.271	2.3	ng/ul	318580	5	21.484	2737840	20.0
(DEL) Alkane: S...	25.573	2.2	ng/ul	340749	6	24.528	3106560	20.0