

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
 Data File : BG062434.D
 Acq On : 16 Aug 2024 3:36
 Operator : MA/JU
 Sample : P3502-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCXT8

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-BG081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062434.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.418	19	22	26	rVB5	5826	7542	0.56%	0.057%
2	3.829	89	92	99	rBV5	9601	16316	1.21%	0.123%
3	3.935	106	110	115	rVB4	8332	12253	0.91%	0.092%
4	4.005	120	122	127	rVB6	3427	5501	0.41%	0.041%
5	4.123	139	142	146	rBV4	2550	3607	0.27%	0.027%
6	4.164	146	149	153	rVB4	3165	3702	0.28%	0.028%
7	4.375	181	185	191	rVB	19460	27862	2.07%	0.210%
8	4.787	249	255	261	rVB2	12886	20151	1.50%	0.152%
9	5.069	298	303	310	rBV2	5540	8970	0.67%	0.067%
10	5.157	313	318	322	rBV5	3522	5920	0.44%	0.045%
11	6.044	464	469	473	rBV3	3698	6594	0.49%	0.050%
12	6.220	495	499	503	rVB5	1598	2854	0.21%	0.021%
13	7.113	644	651	660	rBV	95826	172317	12.83%	1.296%
14	7.283	672	680	687	rVV	65101	105891	7.88%	0.796%
15	7.489	708	715	722	rVB	81356	135205	10.07%	1.017%
16	7.953	788	794	801	rBV	239107	402814	29.99%	3.030%
17	8.018	801	805	810	rVB3	2872	4910	0.37%	0.037%
18	8.652	902	913	922	rBV	91203	153211	11.41%	1.152%
19	8.769	928	933	943	rBV2	16600	33649	2.51%	0.253%
20	8.893	948	954	958	rBV5	1329	2724	0.20%	0.020%
21	9.104	983	990	997	rBV	83830	143969	10.72%	1.083%
22	9.668	1080	1086	1092	rVB3	9225	14687	1.09%	0.110%
23	9.827	1106	1113	1120	rVB	63531	111010	8.26%	0.835%
24	9.956	1131	1135	1143	rBV3	5158	10988	0.82%	0.083%
25	10.185	1168	1174	1177	rBV4	2197	3786	0.28%	0.028%
26	10.361	1197	1204	1214	rVB	108614	193256	14.39%	1.454%
27	10.749	1262	1270	1277	rBV	389081	669928	49.87%	5.039%
28	10.878	1284	1292	1299	rBV	61689	111823	8.32%	0.841%
29	11.278	1355	1360	1364	rBV4	6151	7607	0.57%	0.057%
30	11.483	1389	1395	1401	rBV2	28938	52471	3.91%	0.395%
31	11.525	1401	1402	1407	rVB	4564	4203	0.31%	0.032%
32	13.410	1720	1723	1727	rVB2	2621	3437	0.26%	0.026%
33	13.904	1805	1807	1813	rBV	2403	3222	0.24%	0.024%
34	13.980	1813	1820	1826	rVV	210131	302985	22.56%	2.279%
35	14.227	1855	1862	1863	rBV3	4565	6696	0.50%	0.050%
36	14.268	1863	1869	1877	rVV	254054	395859	29.47%	2.977%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
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37	14.485	1901	1906	1910	rBV3	2633	4656	0.35%	0.035%
38	14.573	1910	1921	1928	rVV	655837	1006460	74.93%	7.570%
39	14.755	1941	1952	1957	rBV	66196	129573	9.65%	0.975%
40	14.820	1962	1963	1971	rVV4	1879	3226	0.24%	0.024%

41	14.908	1973	1978	1984	rVB5	3151	5296	0.39%	0.040%
42	14.985	1986	1991	1997	rBV6	6525	11060	0.82%	0.083%
43	15.308	2043	2046	2050	rVB3	2862	3767	0.28%	0.028%
44	15.378	2054	2058	2064	rVB4	2199	3336	0.25%	0.025%
45	15.431	2064	2067	2069	rBV2	3154	3032	0.23%	0.023%

46	15.566	2083	2090	2096	rBV	340798	521274	38.81%	3.921%
47	15.672	2103	2108	2116	rVV	54849	82269	6.12%	0.619%
48	16.218	2198	2201	2209	rVB7	5128	8742	0.65%	0.066%
49	16.295	2209	2214	2216	rBV4	4719	5138	0.38%	0.039%
50	16.318	2216	2218	2223	rVB4	3233	3414	0.25%	0.026%

51	16.424	2232	2236	2238	rBV4	2183	2963	0.22%	0.022%
52	16.447	2238	2240	2244	rVV5	3721	3537	0.26%	0.027%
53	16.718	2283	2286	2290	rVV4	4800	5579	0.42%	0.042%
54	16.870	2306	2312	2317	rBV6	4985	9509	0.71%	0.072%
55	16.923	2317	2321	2323	rBV4	3381	4205	0.31%	0.032%

56	16.964	2323	2328	2334	rVB4	17396	26554	1.98%	0.200%
57	17.082	2344	2348	2352	rBV5	6138	8771	0.65%	0.066%
58	17.135	2354	2357	2362	rVB5	3705	5881	0.44%	0.044%
59	17.217	2367	2371	2372	rBV4	3766	5223	0.39%	0.039%
60	17.311	2378	2387	2393	rBV	780985	1187970	88.44%	8.935%

61	17.411	2398	2404	2409	rVV2	354609	551518	41.06%	4.148%
62	17.446	2409	2410	2414	rVV	45299	35164	2.62%	0.264%
63	17.475	2414	2415	2421	rVB5	2877	3386	0.25%	0.025%
64	17.587	2432	2434	2438	rBV5	3801	5889	0.44%	0.044%
65	17.710	2452	2455	2459	rVB	10594	15329	1.14%	0.115%

66	17.822	2469	2474	2477	rBV5	5839	8982	0.67%	0.068%
67	17.980	2499	2501	2507	rVB6	4718	6683	0.50%	0.050%
68	18.092	2514	2520	2525	rBV3	23095	39927	2.97%	0.300%
69	18.151	2525	2530	2535	rVV	39827	56451	4.20%	0.425%
70	18.210	2535	2540	2549	rBV	182972	272538	20.29%	2.050%

71	18.515	2587	2592	2596	rBV4	12024	23301	1.73%	0.175%
72	18.721	2623	2627	2631	rBV7	6628	8421	0.63%	0.063%
73	18.774	2633	2636	2642	rVB4	8967	12682	0.94%	0.095%
74	18.938	2660	2664	2667	rVB5	7146	9467	0.70%	0.071%
75	19.003	2671	2675	2680	rVB7	7527	12296	0.92%	0.092%

76	19.044	2680	2682	2683	rBV2	3536	3382	0.25%	0.025%
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Integrator: RTE

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Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

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 Title : SVOA CALIBRATION

77	19.091	2687	2690	2695	rVB7	12634	18295	1.36%	0.138%
78	19.144	2695	2699	2702	rBV	15137	23463	1.75%	0.176%
79	19.332	2728	2731	2733	rBV4	23233	30136	2.24%	0.227%
80	19.361	2733	2736	2744	rVV	56148	97049	7.22%	0.730%
81	19.420	2744	2746	2752	rVB4	16568	19683	1.47%	0.148%
82	19.478	2752	2756	2766	rBV	72175	121509	9.05%	0.914%
83	19.696	2787	2793	2797	rBV	454958	781131	58.15%	5.875%
84	19.860	2819	2821	2825	rBV4	13645	13056	0.97%	0.098%
85	19.960	2836	2838	2841	rBV4	7050	5269	0.39%	0.040%
86	20.142	2867	2869	2872	rBV3	7682	7941	0.59%	0.060%
87	20.248	2884	2887	2892	rVB	29332	36826	2.74%	0.277%
88	20.324	2898	2900	2905	rBV6	10949	10018	0.75%	0.075%
89	20.741	2967	2971	2974	rVB	31630	35664	2.66%	0.268%
90	21.229	3049	3054	3059	rBV3	121410	206326	15.36%	1.552%
91	21.464	3089	3094	3102	rBV	157174	225583	16.79%	1.697%
92	21.552	3103	3109	3115	rBV2	795533	1310703	97.58%	9.858%
93	21.769	3142	3146	3153	rVB2	41004	67156	5.00%	0.505%
94	22.363	3243	3247	3257	rVB3	67011	146133	10.88%	1.099%
95	23.802	3486	3492	3497	rBV	101832	198254	14.76%	1.491%
96	24.431	3591	3599	3614	rVB2	197654	554162	41.26%	4.168%
97	24.642	3626	3635	3643	rBV	504844	1343251	100.00%	10.103%
98	25.799	3824	3832	3842	rVB2	91347	262567	19.55%	1.975%
99	27.080	4043	4050	4063	rVB6	86904	306878	22.85%	2.308%
100	28.660	4312	4319	4331	rVB6	48592	190074	14.15%	1.430%

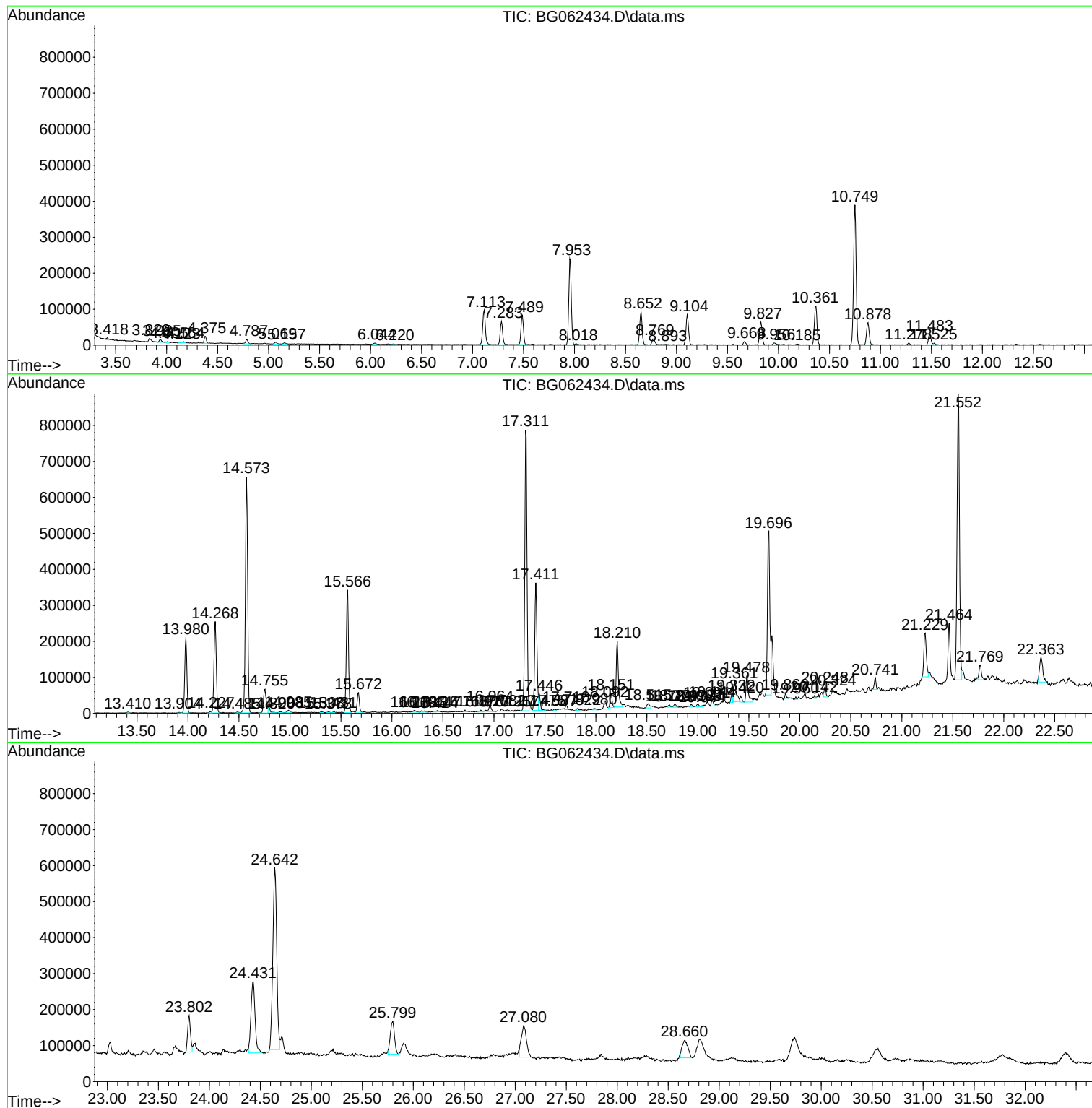
Sum of corrected areas: 13295898

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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



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Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCXT8

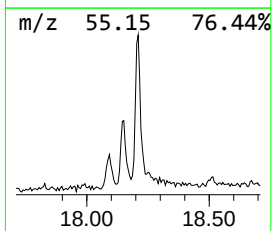
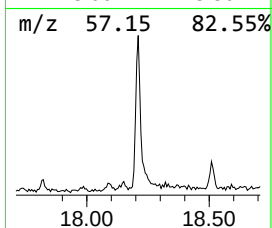
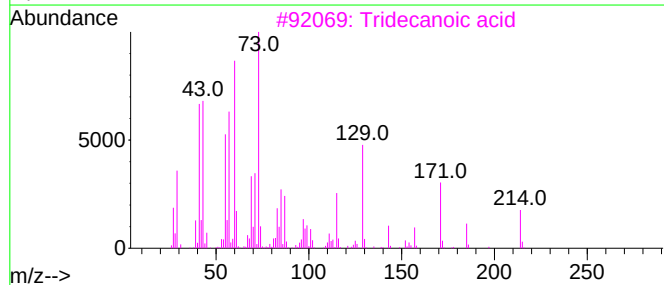
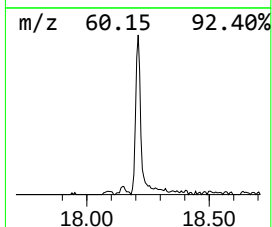
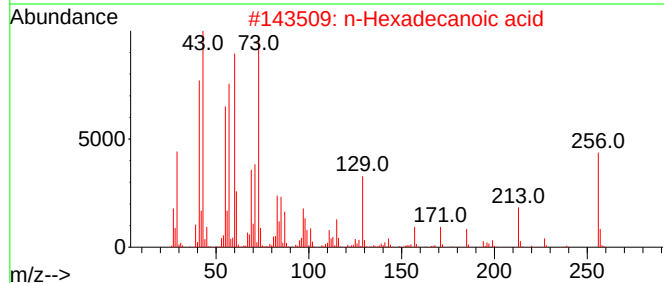
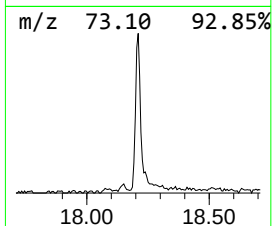
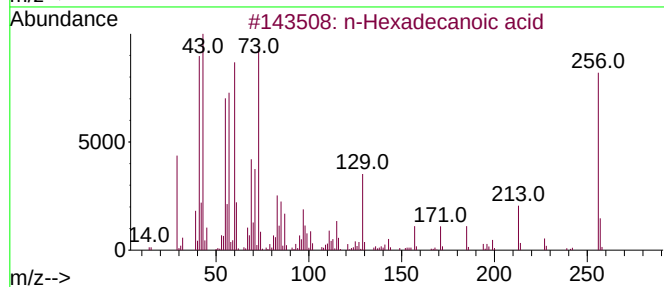
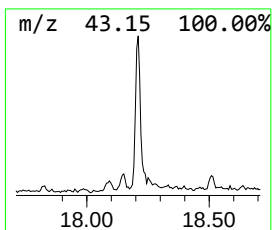
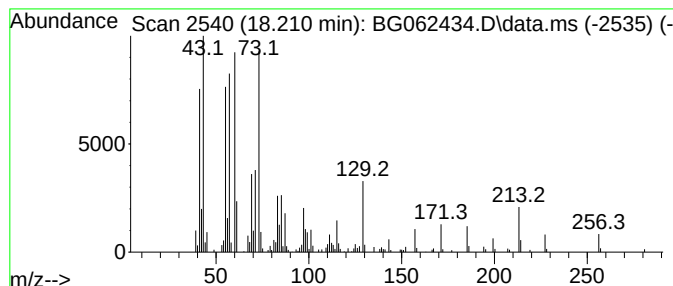
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	4.59 ng/ul	272538	Phenanthrene-d10	17.311

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
5			n-Decanoic acid	172	C10H20O2	000334-48-5	91



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Data File : BG062434.D
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Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

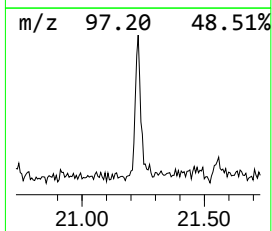
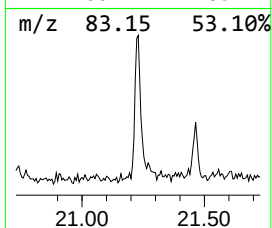
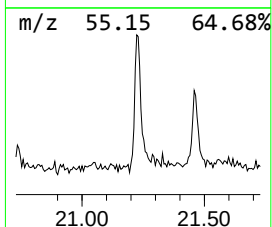
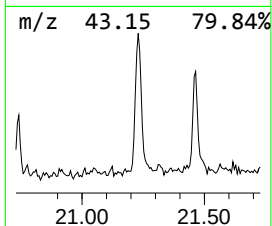
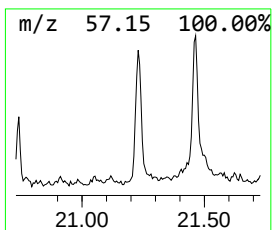
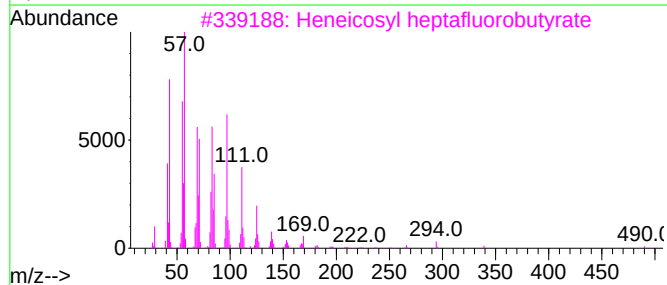
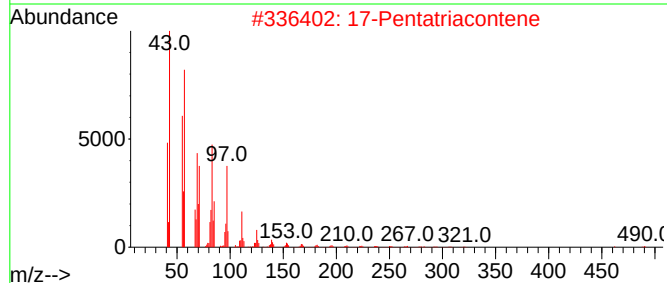
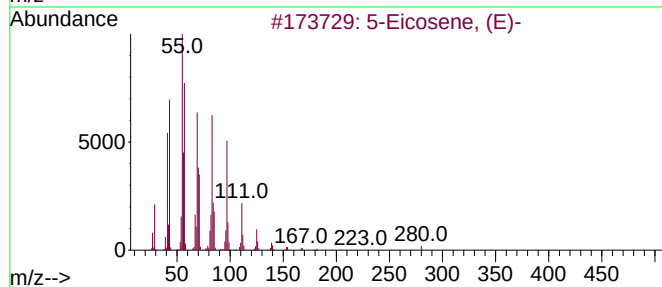
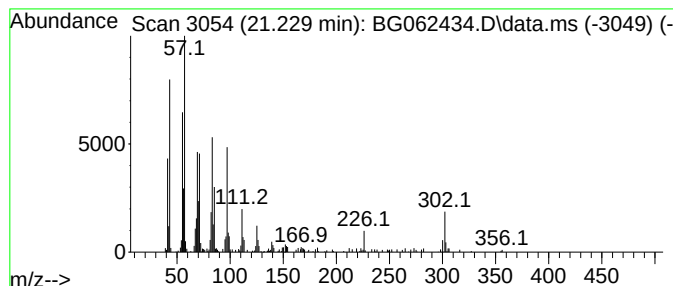
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.229	3.15 ng/ul	206326	Chrysene-d12		21.552	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	87
2	17-Pentatriacontene		491	C35H70	006971-40-0	87
3	Heneicosyl heptafluorobutyrate		508	C25H43F7O2	1000351-83-8	87
4	1-Hexadecanesulfonyl chloride		324	C16H33ClO2S	038775-38-1	83
5	Triacontyl heptafluorobutyrate		634	C34H61F7O2	1000351-83-2	83



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Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DCXT8

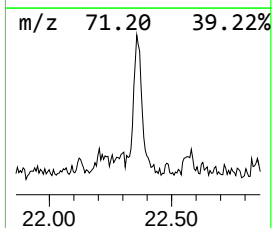
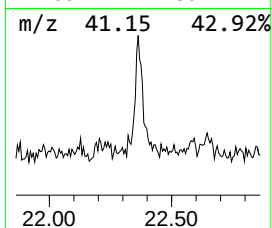
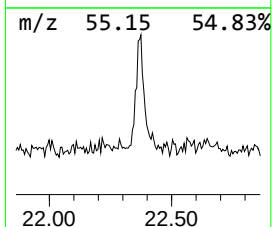
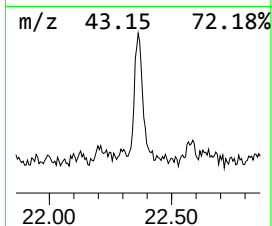
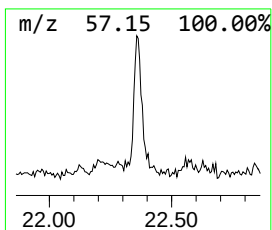
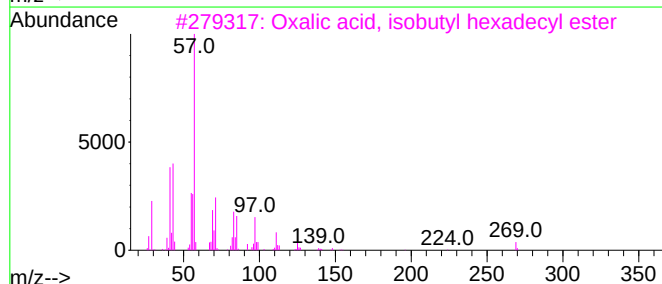
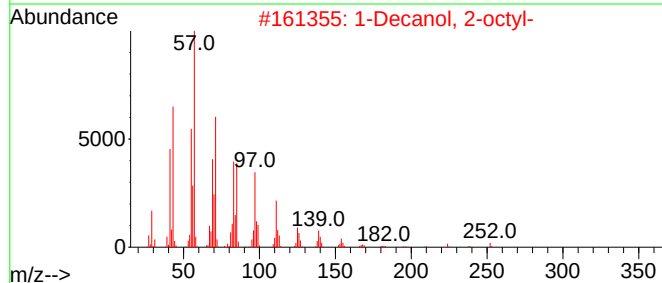
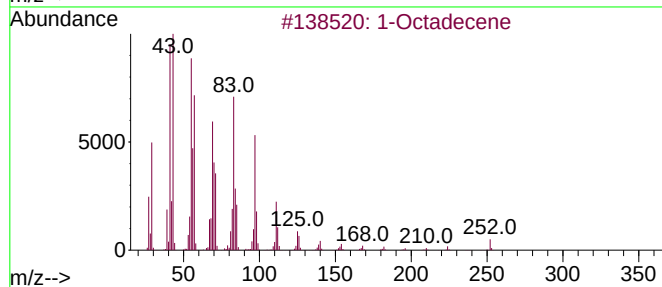
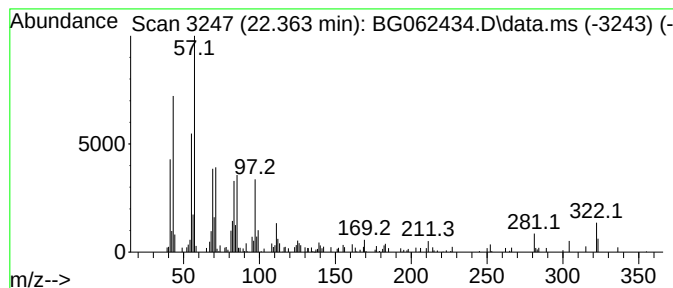
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.363	2.23 ng/ul	146133	Chrysene-d12	21.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	70
2			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	68
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	68
4			Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	68
5			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
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Acq On : 16 Aug 2024 3:36
Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

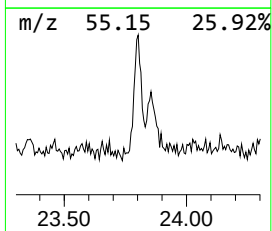
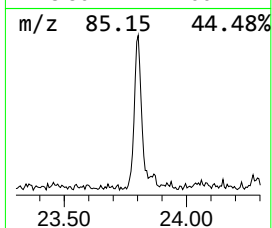
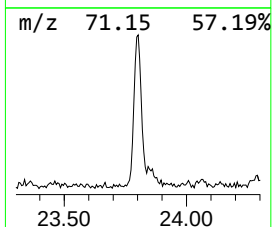
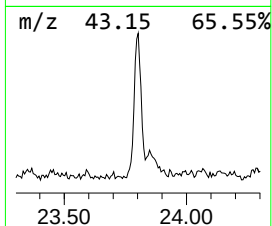
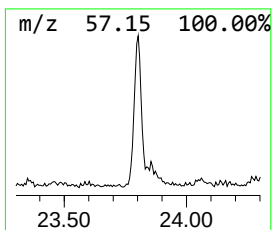
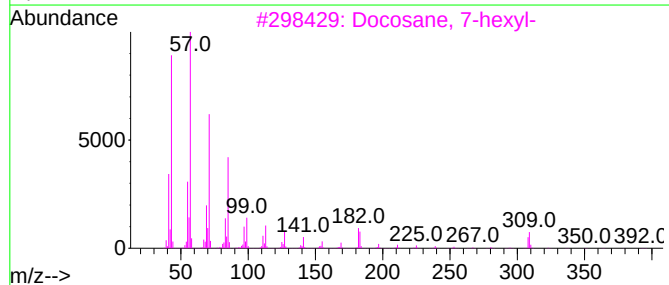
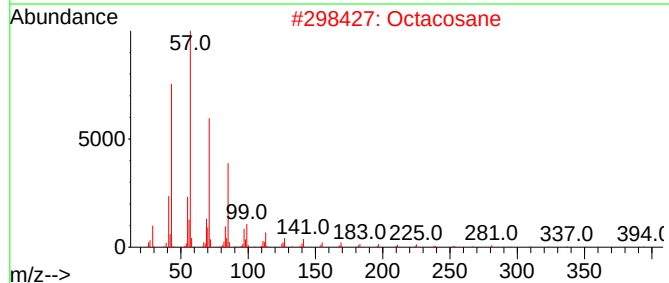
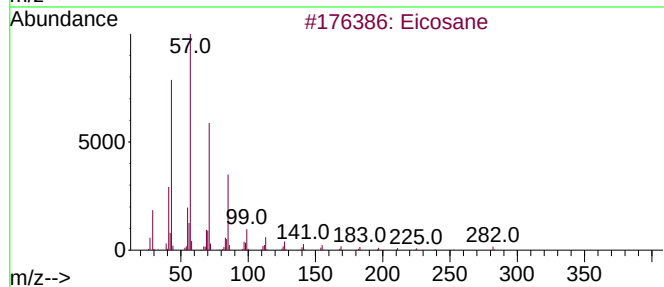
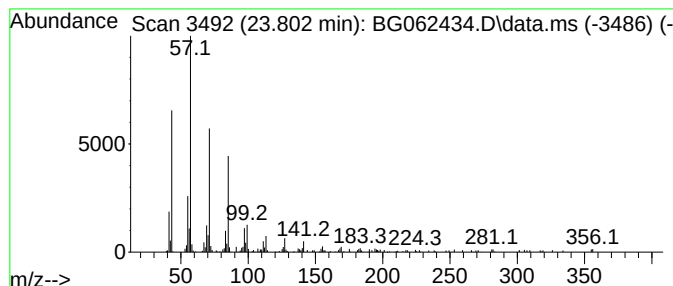
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.802	2.95 ng/ul	198254	Perylene-d12		24.642	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Octacosane		394	C28H58	000630-02-4	90
3	Docosane, 7-hexyl-		394	C28H58	055373-86-9	87
4	Eicosane		282	C20H42	000112-95-8	87
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062434.D
Acq On : 16 Aug 2024 3:36
Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCXT8

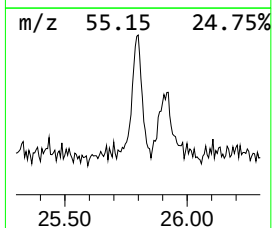
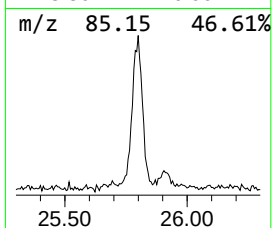
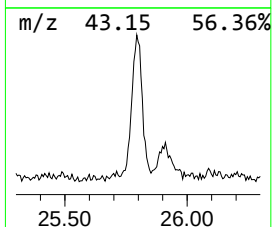
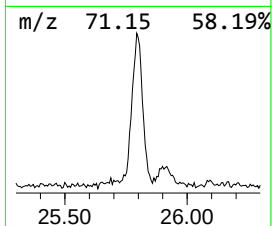
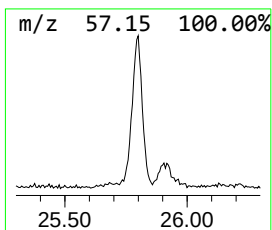
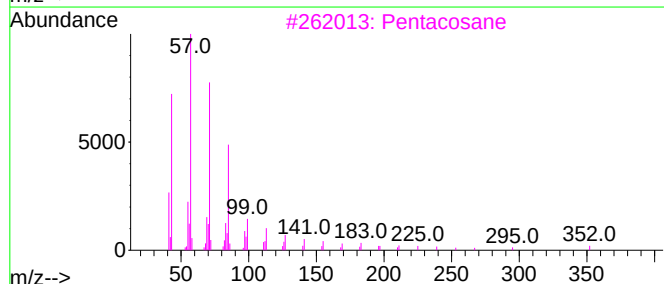
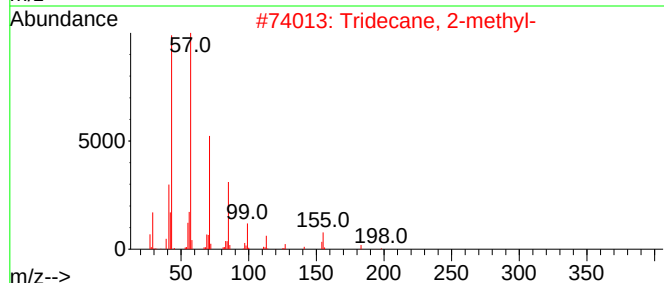
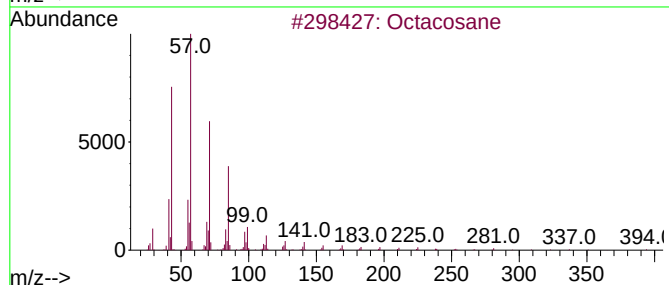
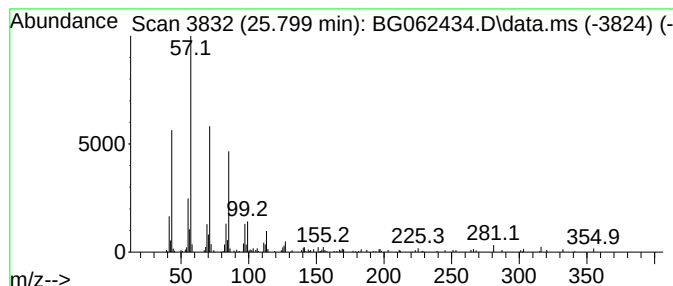
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Quant Title : SVOA CALIBRATION

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.
25.799	3.91 ng/ul	262567	Perylene-d12	24.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
3			Pentacosane	352	C25H52	000629-99-2	86
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062434.D
Acq On : 16 Aug 2024 3:36
Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

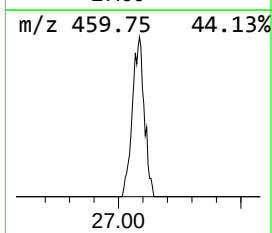
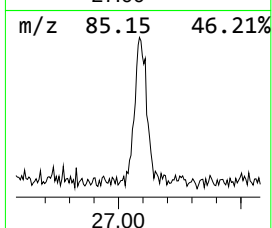
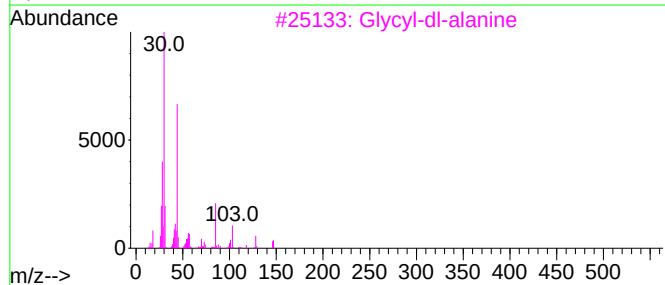
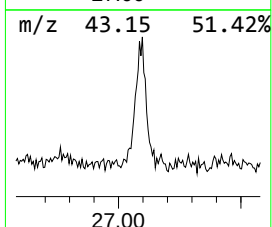
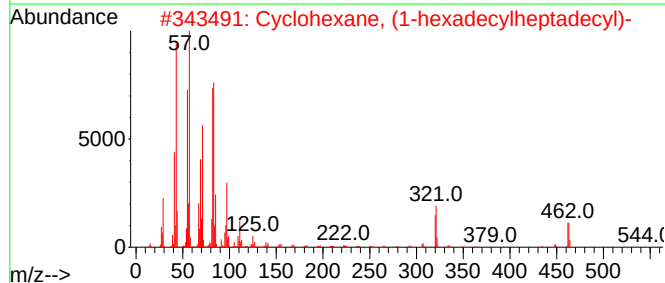
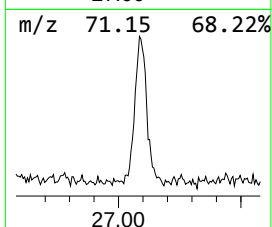
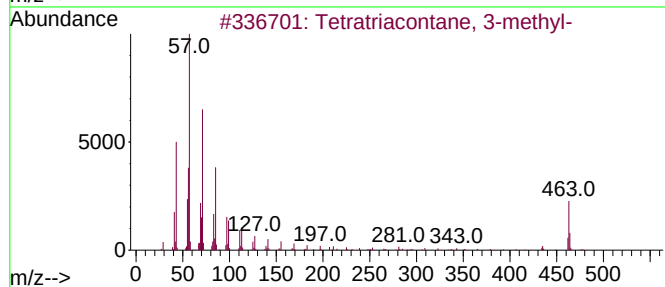
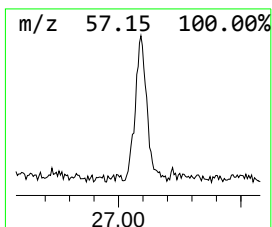
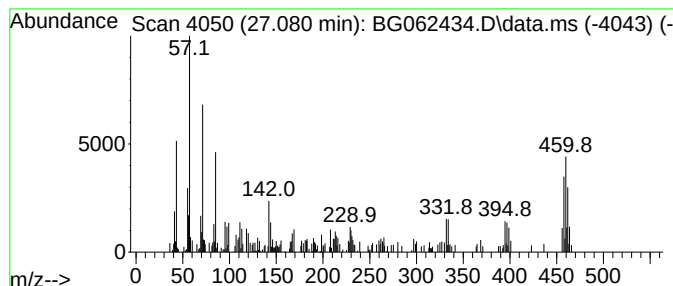
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
27.080	4.57 ng/ul	306878	Perylene-d12		24.642	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetratriacontane, 3-methyl-		493	C35H72	066309-88-4	10
2	Cyclohexane, (1-hexadecylheptade...		547	C39H78	055517-75-4	7
3	Glycyl-dl-alanine		146	C5H10N2O3	000926-77-2	4
4	N,N'-Diacetylenediamine		144	C6H12N2O2	000871-78-3	4
5	3-Debenzoyl-tetrahydrocarpesterol		462	C30H54O3	1000214-22-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062434.D
Acq On : 16 Aug 2024 3:36
Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

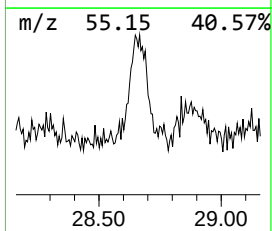
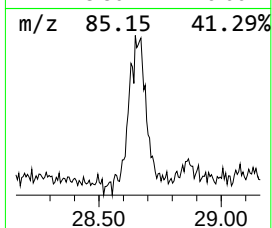
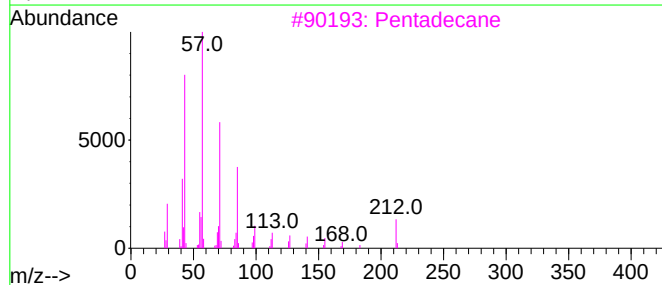
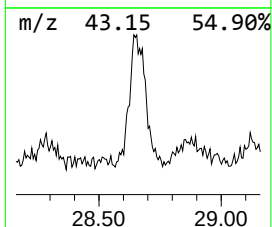
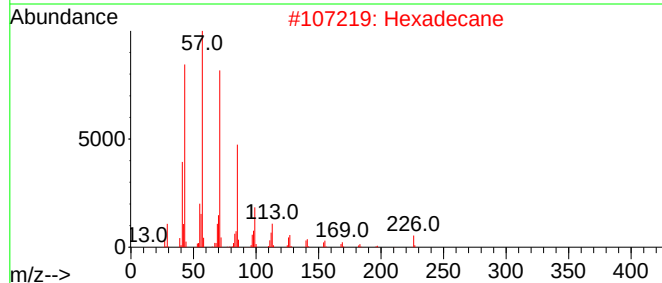
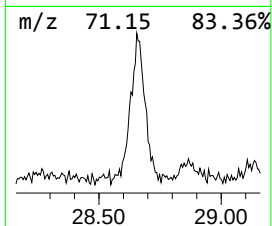
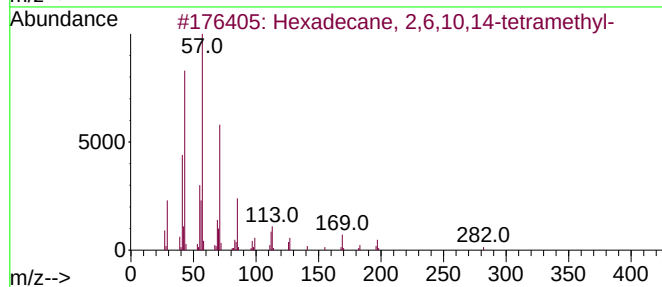
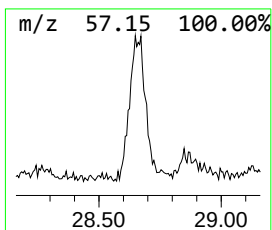
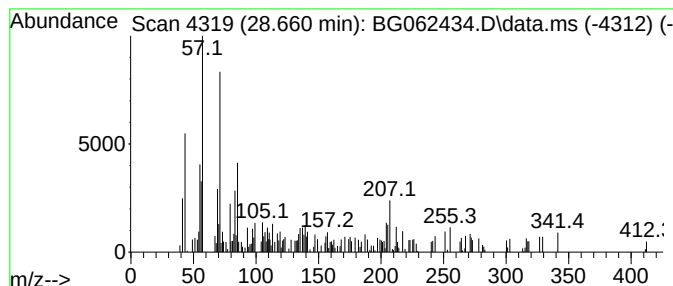
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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.	
28.660	2.83 ng/ul	190074	Perylene-d12	24.642	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
2	Hexadecane	226	C16H34	000544-76-3	64
3	Pentadecane	212	C15H32	000629-62-9	62
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	58
5	Pentadecane	212	C15H32	000629-62-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062434.D
Acq On : 16 Aug 2024 3:36
Operator : MA/JU
Sample : P3502-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCXT8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.210	4.6	ng/ul	272538	4	17.311	1187970	20.0
(DEL) Alkane: S...	21.229	3.1	ng/ul	206326	5	21.552	1310700	20.0
(DEL) Alkane: S...	22.363	2.2	ng/ul	146133	5	21.552	1310700	20.0
(DEL) Alkane: S...	23.802	3.0	ng/ul	198254	6	24.642	1343250	20.0
(DEL) Alkane: S...	25.799	3.9	ng/ul	262567	6	24.642	1343250	20.0
(DEL) Alkane: S...	27.080	4.6	ng/ul	306878	6	24.642	1343250	20.0
(DEL) Alkane: S...	28.660	2.8	ng/ul	190074	6	24.642	1343250	20.0