

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
 Data File : BG062488.D
 Acq On : 20 Aug 2024 22:42
 Operator : MA/JU
 Sample : P3504-14
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCYE6

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: BG062488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.408	17	20	24	rVB3	14133	17104	1.00%	0.078%
2	3.666	60	64	71	rBV	37037	57639	3.37%	0.264%
3	3.813	85	89	99	rBV	67604	105113	6.15%	0.481%
4	4.148	143	146	154	rVB5	4796	8018	0.47%	0.037%
5	5.059	296	301	304	rBV4	2819	5118	0.30%	0.023%
6	6.028	461	466	474	rVB2	7109	12676	0.74%	0.058%
7	6.204	492	496	500	rBV4	2974	4467	0.26%	0.020%
8	6.369	519	524	530	rVB4	4255	6919	0.41%	0.032%
9	6.639	565	570	575	rBV2	20976	32989	1.93%	0.151%
10	7.103	642	649	659	rBV	281482	486619	28.48%	2.226%
11	7.267	670	677	687	rBV	184551	311697	18.25%	1.426%
12	7.473	705	712	719	rBV	256549	422394	24.73%	1.932%
13	7.532	719	722	729	rVB	8771	12772	0.75%	0.058%
14	7.943	785	792	799	rBV	351928	601970	35.24%	2.753%
15	8.002	799	802	807	rVB4	6118	8917	0.52%	0.041%
16	8.636	904	910	920	rBV	333693	561369	32.86%	2.568%
17	9.094	979	988	997	rBV	235580	428835	25.10%	1.961%
18	9.171	997	1001	1005	rVV5	4553	8550	0.50%	0.039%
19	9.535	1057	1063	1068	rBV3	4025	7259	0.42%	0.033%
20	9.652	1077	1083	1090	rVV3	24710	41798	2.45%	0.191%
21	9.811	1103	1110	1120	rBV	202923	356319	20.86%	1.630%
22	10.040	1144	1149	1150	rBV3	2805	4294	0.25%	0.020%
23	10.351	1194	1202	1213	rBV	350078	608009	35.59%	2.781%
24	10.510	1224	1229	1235	rVB3	3152	5844	0.34%	0.027%
25	10.733	1258	1267	1276	rBV	559800	977939	57.25%	4.473%
26	10.863	1279	1289	1301	rBV	79582	151051	8.84%	0.691%
27	11.262	1352	1357	1362	rBV2	8874	13012	0.76%	0.060%
28	11.468	1385	1392	1406	rBV	50310	100658	5.89%	0.460%
29	11.614	1412	1417	1423	rBV2	5075	10188	0.60%	0.047%
30	12.313	1532	1536	1541	rVB3	6258	8689	0.51%	0.040%
31	13.394	1714	1720	1724	rVV4	3265	5847	0.34%	0.027%
32	13.453	1726	1730	1737	rVV5	6339	12048	0.71%	0.055%
33	13.529	1737	1743	1746	rVV2	2690	4290	0.25%	0.020%
34	13.894	1800	1805	1811	rVV2	42865	61253	3.59%	0.280%
35	13.964	1811	1817	1824	rBV	497060	721021	42.21%	3.298%
36	14.099	1835	1840	1843	rBV4	3775	5384	0.32%	0.025%

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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
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37	14.252	1859	1866	1877	rVB2	602361	932330	54.58%	4.264%
38	14.411	1887	1893	1898	rBV5	6388	10027	0.59%	0.046%
39	14.558	1908	1918	1926	rBV	769486	1221934	71.53%	5.589%
40	14.634	1926	1931	1937	rVB4	9998	14242	0.83%	0.065%
41	14.745	1943	1950	1960	rBV2	200243	379682	22.23%	1.737%
42	14.969	1985	1988	1990	rBV3	4076	4929	0.29%	0.023%
43	15.356	2050	2054	2055	rBV2	3757	4460	0.26%	0.020%
44	15.415	2059	2064	2067	rBV4	4026	5900	0.35%	0.027%
45	15.468	2067	2073	2080	rBV7	6422	12030	0.70%	0.055%
46	15.550	2080	2087	2098	rVB	790735	1163876	68.13%	5.323%
47	15.656	2099	2105	2112	rBV	182624	267908	15.68%	1.225%
48	15.791	2124	2128	2132	rBV4	3643	5440	0.32%	0.025%
49	15.985	2155	2161	2164	rBV3	6513	10805	0.63%	0.049%
50	16.026	2164	2168	2174	rVB6	5054	9242	0.54%	0.042%
51	16.126	2178	2185	2188	rBV7	4962	8013	0.47%	0.037%
52	16.279	2204	2211	2215	rVV5	5114	9005	0.53%	0.041%
53	16.402	2228	2232	2240	rVV6	5528	10115	0.59%	0.046%
54	16.690	2277	2281	2288	rVB9	2671	5900	0.35%	0.027%
55	16.854	2305	2309	2314	rBV6	4297	8362	0.49%	0.038%
56	17.072	2342	2346	2348	rBV4	4191	5699	0.33%	0.026%
57	17.301	2378	2385	2392	rVV	946373	1426690	83.51%	6.526%
58	17.401	2395	2402	2410	rVB	732144	1109487	64.95%	5.075%
59	17.524	2416	2423	2427	rBV8	3386	7790	0.46%	0.036%
60	17.971	2497	2499	2504	rBV6	4623	5698	0.33%	0.026%
61	18.194	2531	2537	2548	rBV2	139489	227852	13.34%	1.042%
62	18.382	2563	2569	2579	rBV	173196	280389	16.41%	1.282%
63	18.487	2585	2587	2589	rBV3	3771	4708	0.28%	0.022%
64	18.523	2589	2593	2601	rVB9	10880	24427	1.43%	0.112%
65	18.634	2607	2612	2614	rBV6	3955	6626	0.39%	0.030%
66	18.670	2614	2618	2624	rVB9	10844	18656	1.09%	0.085%
67	18.910	2658	2659	2664	rVB4	5330	5325	0.31%	0.024%
68	19.081	2681	2688	2691	rBV7	13166	26616	1.56%	0.122%
69	19.245	2712	2716	2721	rBV2	12602	20891	1.22%	0.096%
70	19.316	2722	2728	2733	rBV2	17745	35109	2.06%	0.161%
71	19.404	2741	2743	2750	rVB7	5303	6541	0.38%	0.030%
72	19.469	2750	2754	2764	rBV2	40619	72307	4.23%	0.331%
73	19.615	2772	2779	2784	rBV8	12871	24937	1.46%	0.114%
74	19.680	2784	2790	2796	rBV	973464	1403863	82.18%	6.421%
75	19.792	2806	2809	2812	rVB5	6574	7885	0.46%	0.036%
76	19.880	2820	2824	2825	rBV4	5119	6609	0.39%	0.030%

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Integrator: RTE

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 Title : SVOA CALIBRATION

77	20.062	2852	2855	2859	rBV2	20349	26377	1.54%	0.121%
78	20.126	2862	2866	2872	rBV	61085	76991	4.51%	0.352%
79	20.197	2874	2878	2880	rVV4	13114	17776	1.04%	0.081%
80	20.226	2880	2883	2891	rVB7	18544	30202	1.77%	0.138%
81	20.444	2918	2920	2922	rBV3	6087	5299	0.31%	0.024%
82	20.655	2952	2956	2962	rVB	84773	112926	6.61%	0.517%
83	20.720	2962	2967	2971	rBV6	15357	26530	1.55%	0.121%
84	21.025	3015	3019	3024	rBV	48596	75821	4.44%	0.347%
85	21.178	3041	3045	3046	rBV2	25924	33945	1.99%	0.155%
86	21.207	3046	3050	3056	rVB	178475	264201	15.47%	1.208%
87	21.401	3080	3083	3089	rVB8	21228	37949	2.22%	0.174%
88	21.536	3100	3106	3116	rBV2	928459	1540944	90.20%	7.048%
89	21.754	3139	3143	3149	rVB6	34890	62097	3.63%	0.284%
90	21.824	3151	3155	3160	rVB6	31010	46284	2.71%	0.212%
91	21.948	3170	3176	3179	rBV4	22011	40334	2.36%	0.184%
92	22.353	3238	3245	3258	rVB3	120011	259757	15.21%	1.188%
93	23.769	3480	3486	3491	rBV2	60016	121123	7.09%	0.554%
94	23.833	3491	3497	3502	rVV5	26452	58939	3.45%	0.270%
95	24.403	3585	3594	3605	rVB	535615	1385831	81.12%	6.339%
96	24.620	3620	3631	3650	rBV	621561	1708338	100.00%	7.814%
97	25.748	3816	3823	3832	rVB2	85789	227595	13.32%	1.041%
98	25.860	3835	3842	3855	rBV3	83191	270749	15.85%	1.238%
99	28.591	4297	4307	4321	rVB5	73165	291929	17.09%	1.335%
100	29.684	4484	4493	4501	rBV5	37870	140772	8.24%	0.644%

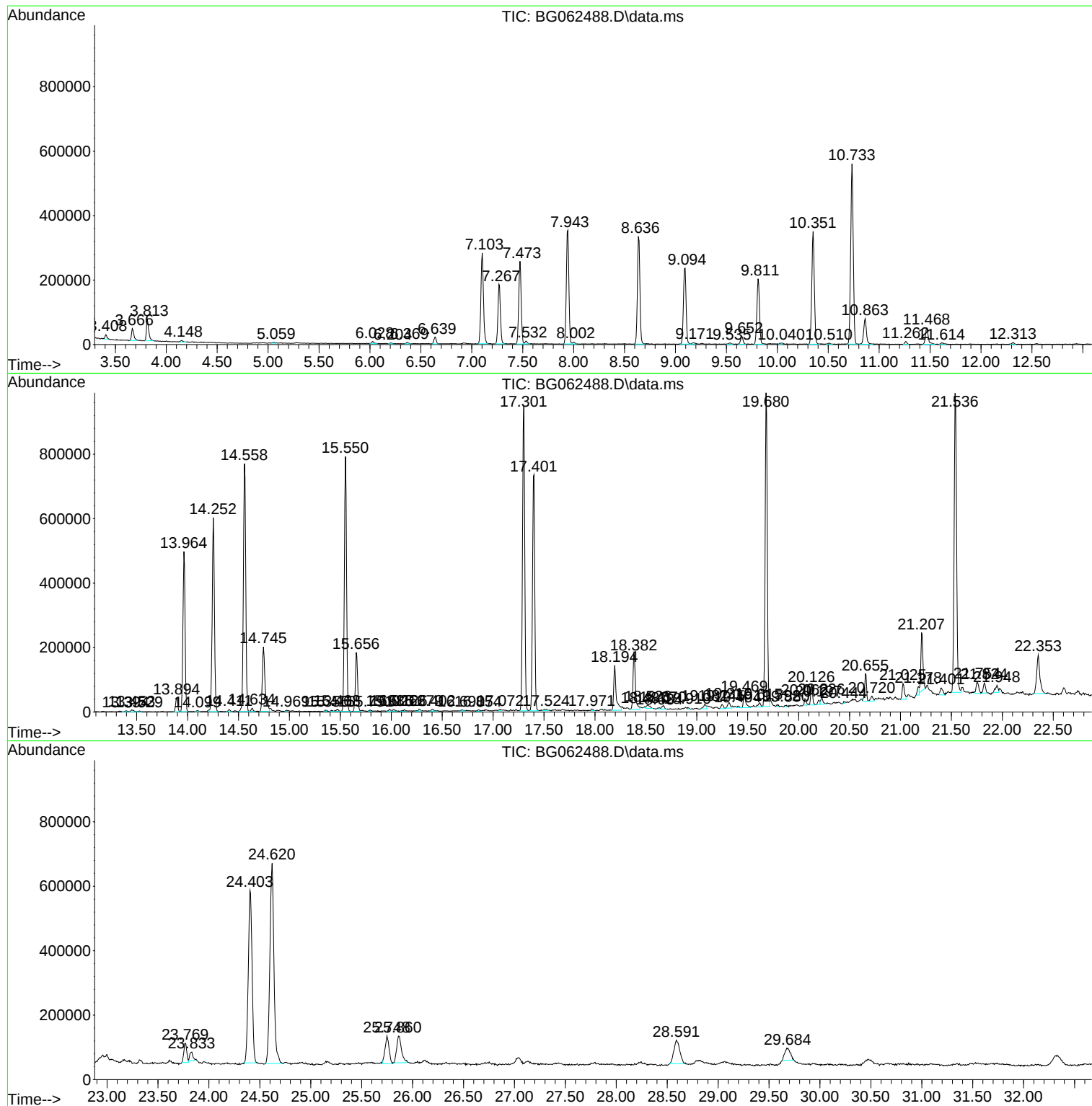
Sum of corrected areas: 21863083

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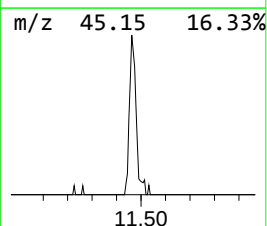
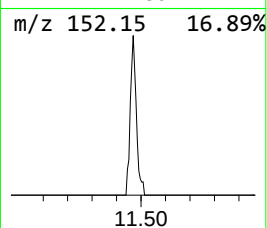
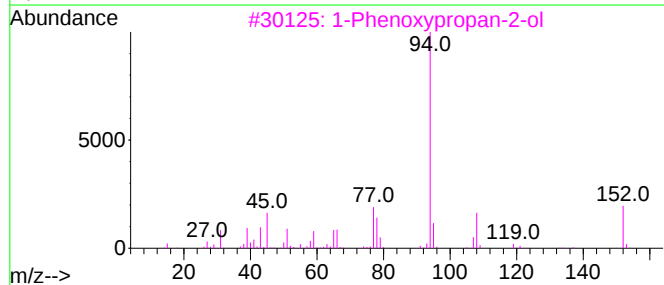
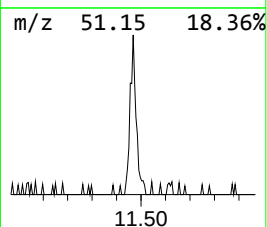
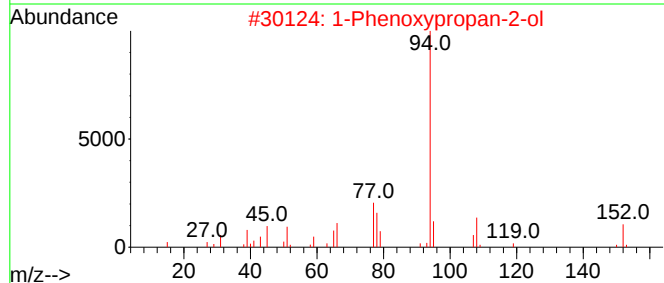
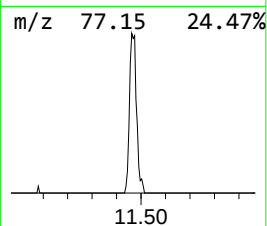
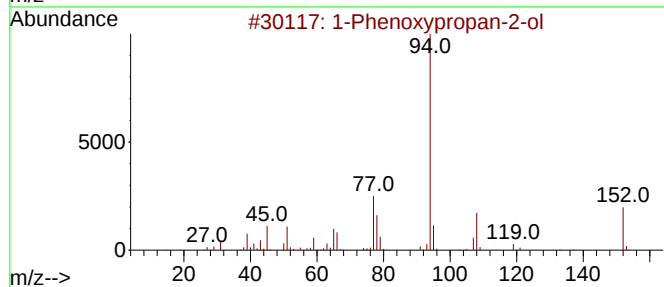
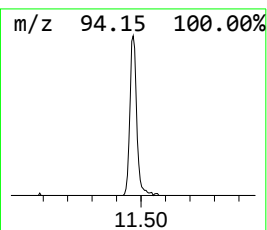
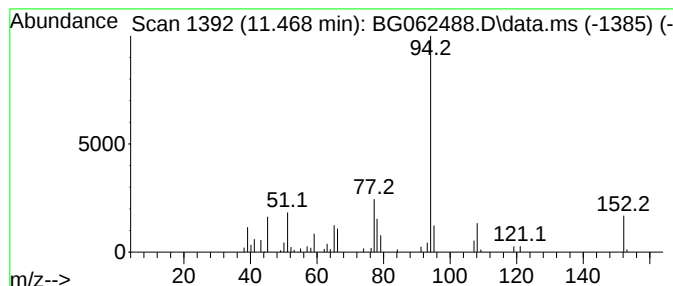
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.468	2.06 ng/ul	100658	Naphthalene-d8	10.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91



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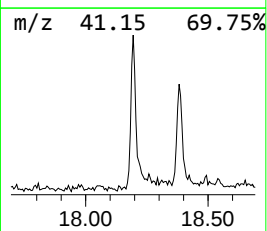
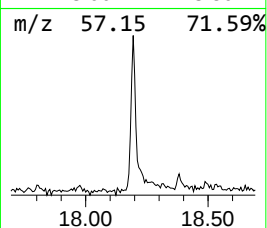
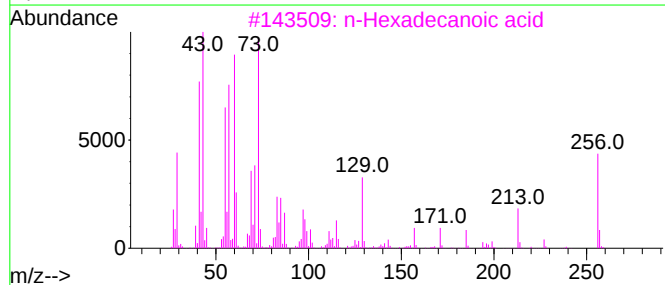
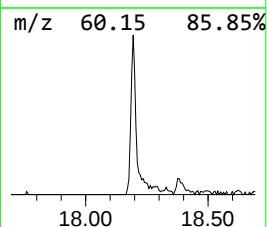
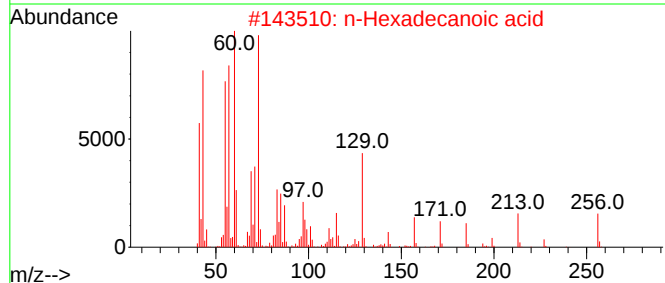
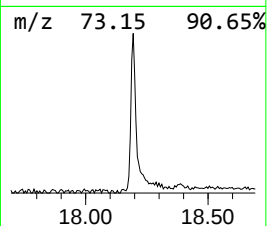
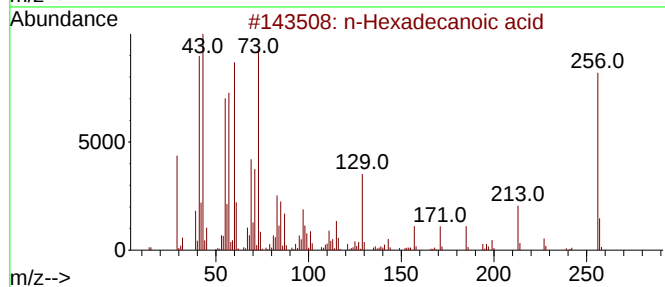
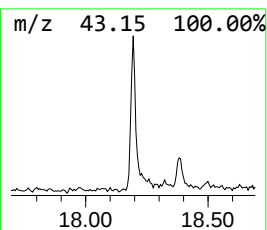
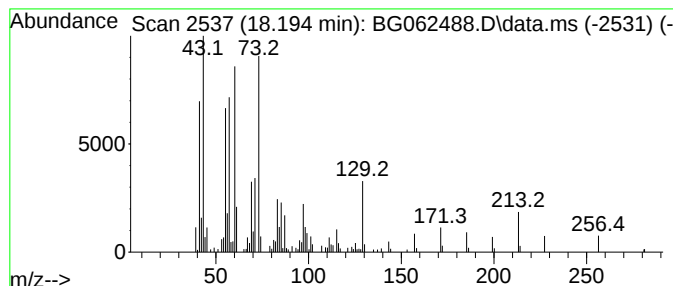
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.194	3.19 ng/ul	227852	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	91



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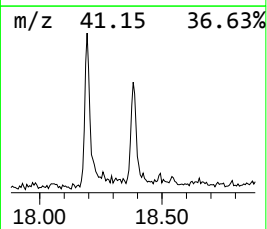
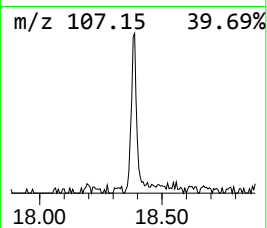
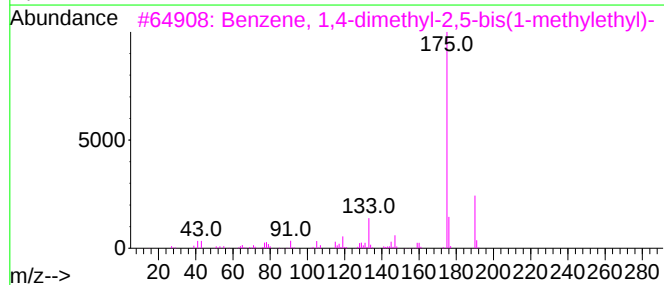
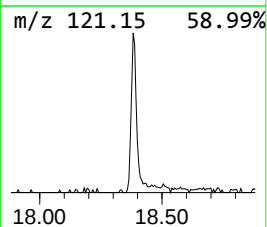
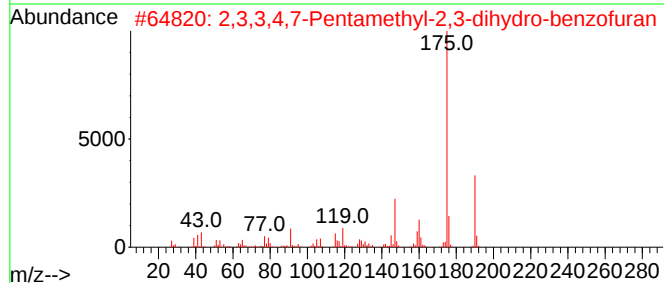
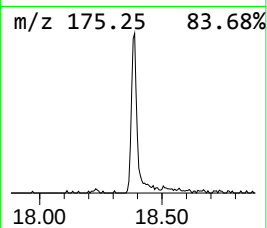
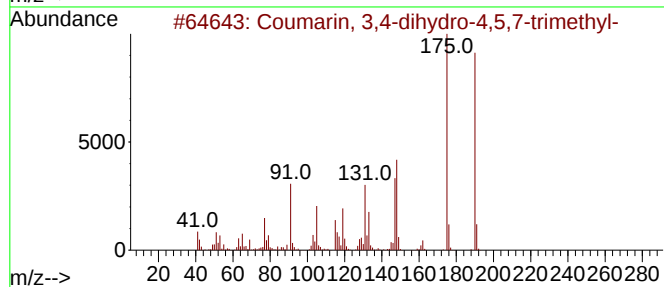
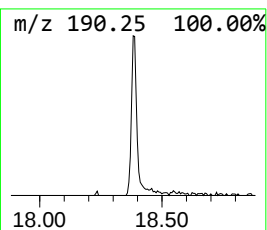
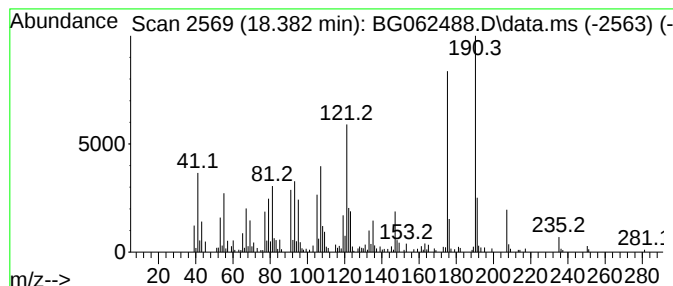
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Coumarin, 3,4-dihydro-4,5,7... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.382	3.93 ng/ul	280389	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Coumarin, 3,4-dihydro-4,5,7-trim...	190	C12H14O2	1000126-60-5	60
2			2,3,3,4,7-Pentamethyl-2,3-dihydr...	190	C13H18O	1000189-42-9	50
3			Benzene, 1,4-dimethyl-2,5-bis(1-...	190	C14H22	010375-96-9	49
4			Phenol, 2-(1,1-dimethyl-2-propen...	190	C13H18O	092617-73-7	49
5			Benzene, 1,2-diethyl-3,4,5,6-tet...	190	C14H22	033884-69-4	49



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Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
Operator : MA/JU
Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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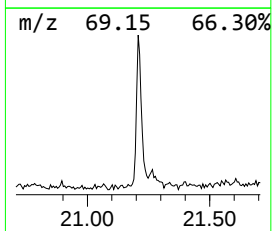
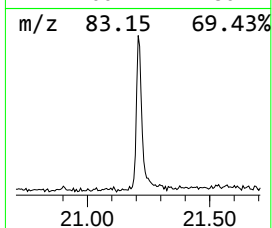
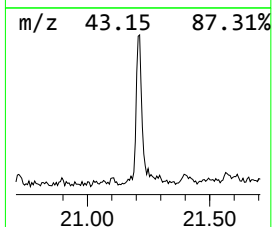
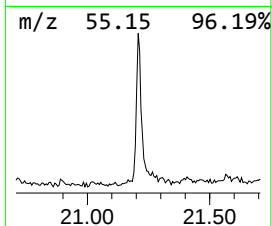
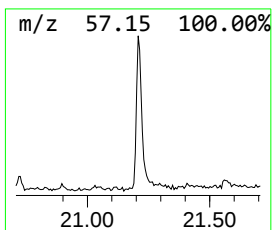
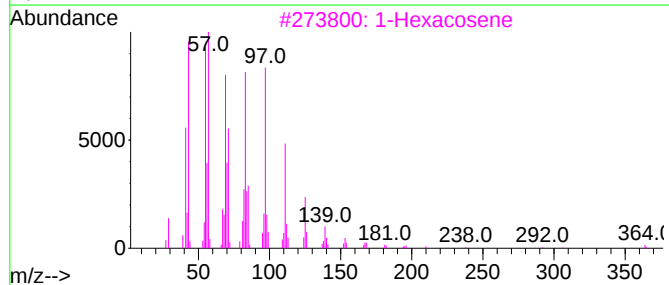
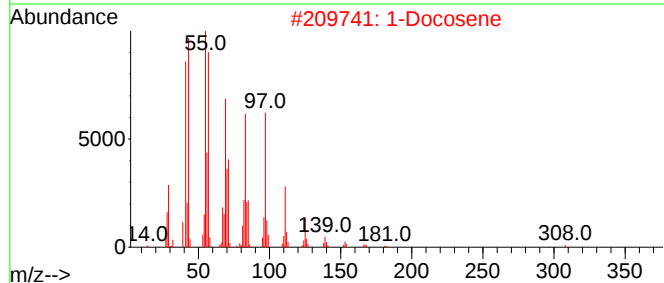
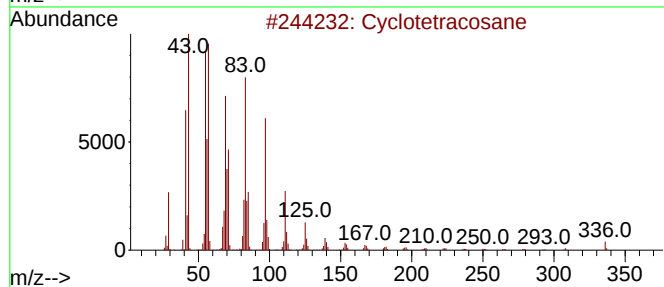
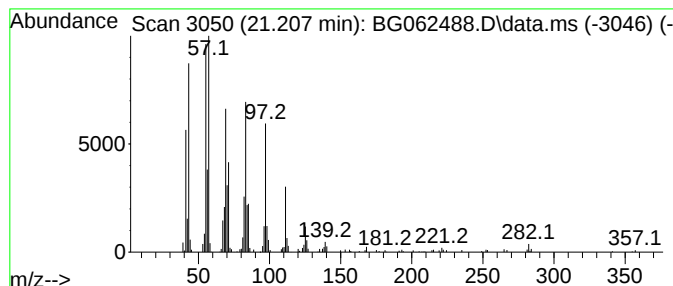
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Cyclic21.207 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.207	3.43 ng/ul	264201	Chrysene-d12	21.536

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			1-Docosene	308	C22H44	001599-67-3	94
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
Operator : MA/JU
Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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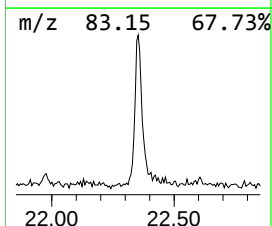
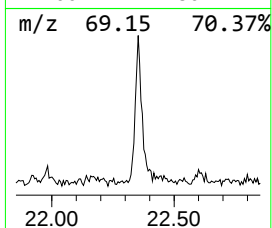
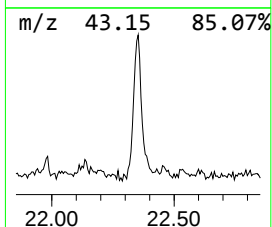
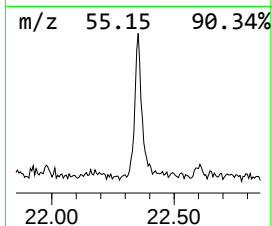
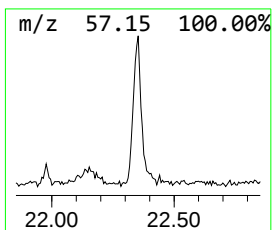
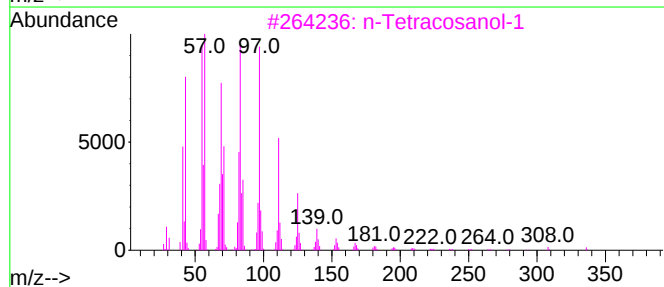
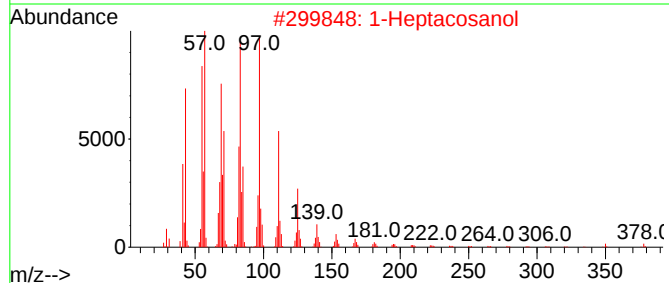
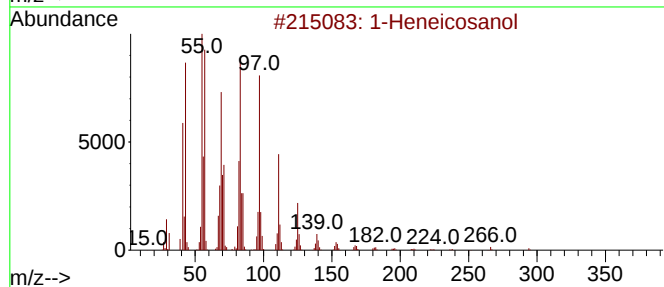
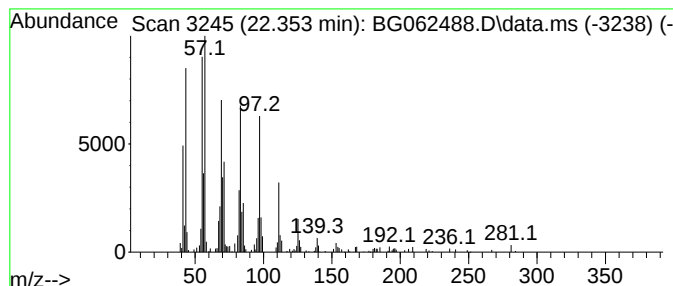
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.353	3.37 ng/ul	259757	Chrysene-d12	21.536

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
Operator : MA/JU
Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

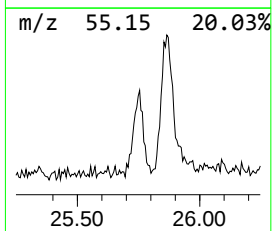
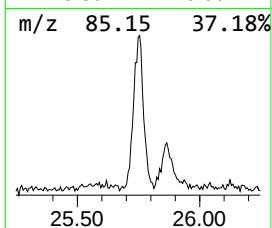
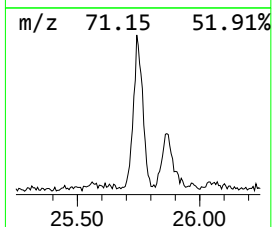
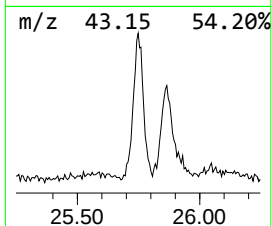
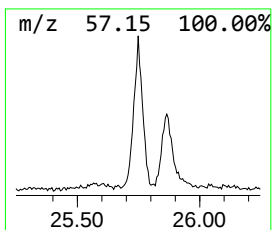
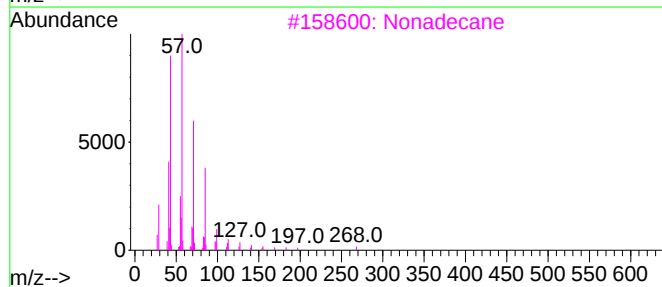
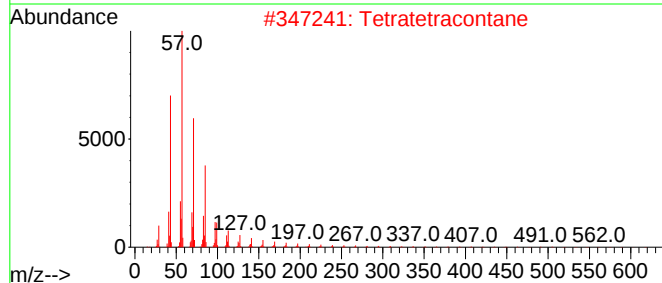
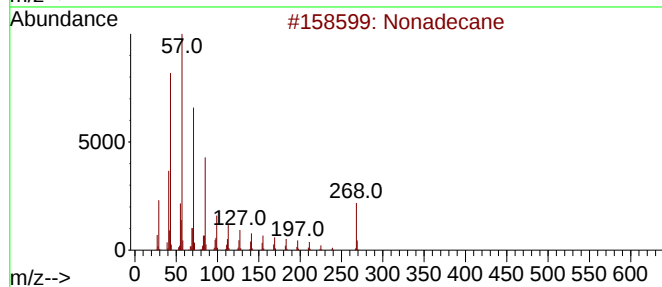
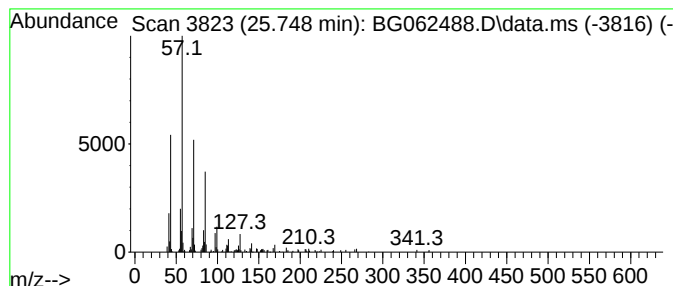
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.748	2.66 ng/ul	227595	Perylene-d12	24.620	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Nonadecane	268	C19H40	000629-92-5	80
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
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Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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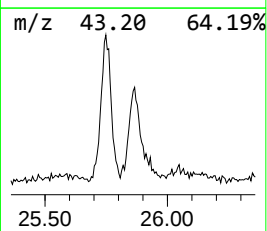
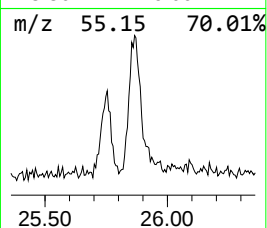
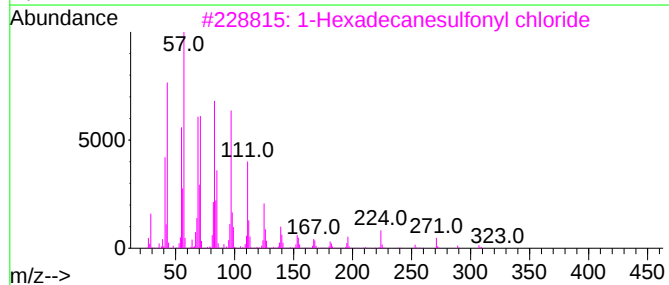
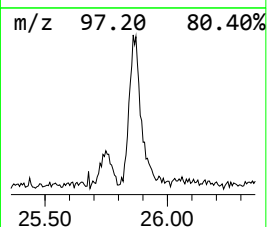
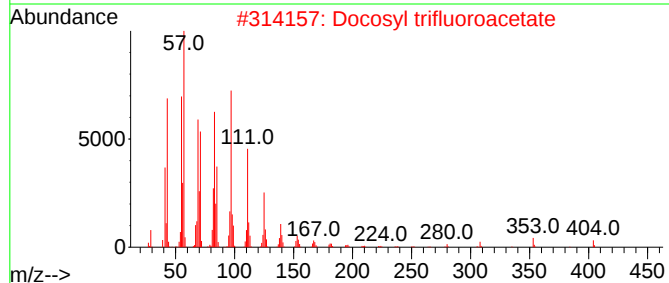
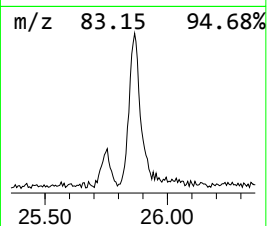
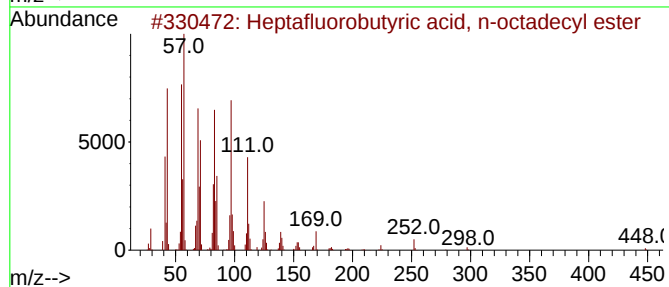
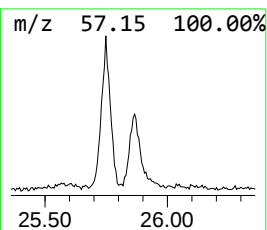
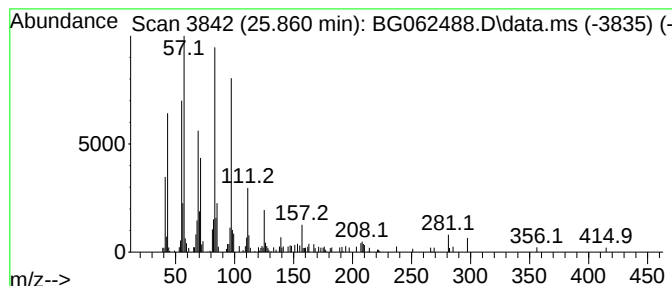
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.860	3.17 ng/ul	270749	Perylene-d12	24.620

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	58
2			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	55
3			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	53
4			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	49
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
Operator : MA/JU
Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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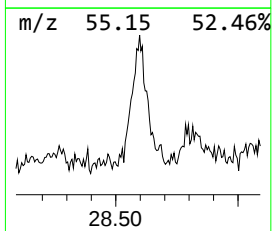
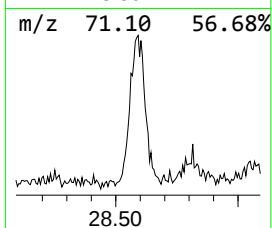
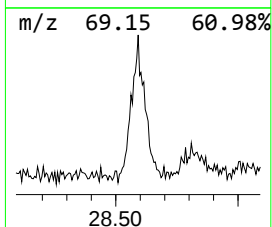
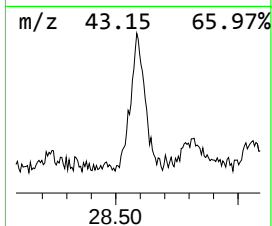
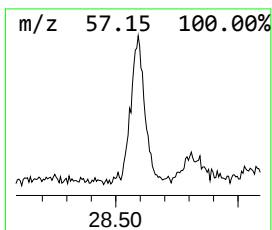
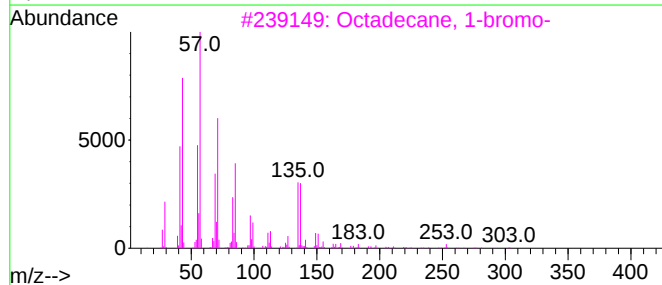
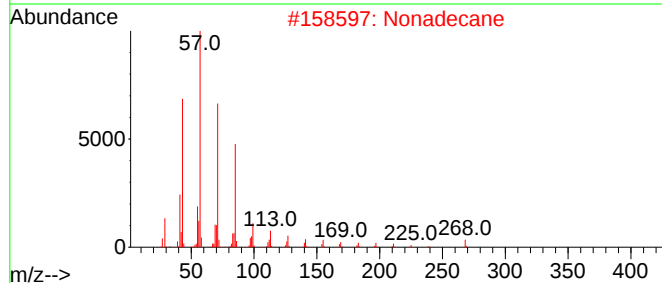
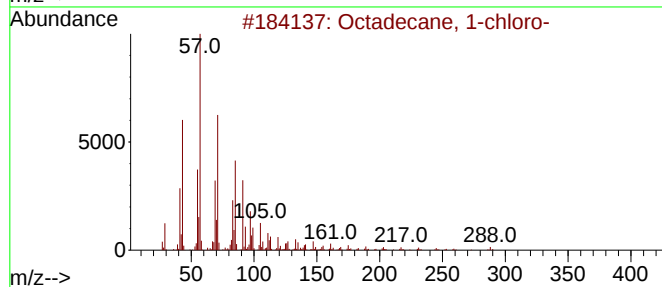
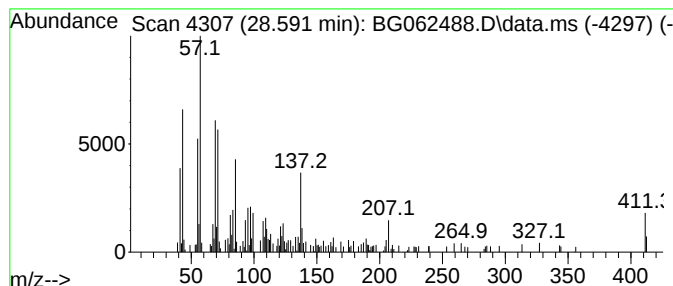
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Octadecane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.591	3.42 ng/ul	291929	Perylene-d12	24.620

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	70
2		Nonadecane	268	C19H40	000629-92-5	60
3		Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	53
4		Nonadecane	268	C19H40	000629-92-5	52
5		Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062488.D
Acq On : 20 Aug 2024 22:42
Operator : MA/JU
Sample : P3504-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Phenoxypropan...	11.468	2.1	ng/ul	100658	2	10.733	977939	20.0
n-Hexadecanoic ...	18.194	3.2	ng/ul	227852	4	17.301	1426690	20.0
Coumarin, 3,4-d...	18.382	3.9	ng/ul	280389	4	17.301	1426690	20.0
(DEL) Alkane: C...	21.207	3.4	ng/ul	264201	5	21.536	1540940	20.0
1-Heneicosanol	22.353	3.4	ng/ul	259757	5	21.536	1540940	20.0
(DEL) Alkane: S...	25.748	2.7	ng/ul	227595	6	24.620	1708340	20.0
Heptafluorobuty...	25.860	3.2	ng/ul	270749	6	24.620	1708340	20.0
Octadecane, 1-c...	28.591	3.4	ng/ul	291929	6	24.620	1708340	20.0