

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
 Data File : BG062247.D
 Acq On : 5 Aug 2024 21:27
 Operator : MA/JU
 Sample : P3361-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E20P0

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-BG080524.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.394	15	18	21	rBV3	6883	9999	0.61%	0.046%
2	3.688	64	68	77	rBV	24882	40674	2.49%	0.186%
3	3.829	88	92	110	rVB	101470	173481	10.61%	0.794%
4	4.169	147	150	155	rVB2	4696	5521	0.34%	0.025%
5	7.112	644	651	663	rVB	188709	320235	19.59%	1.466%
6	7.294	675	682	693	rVB	138718	224678	13.75%	1.029%
7	7.494	709	716	723	rBV	170751	284953	17.43%	1.305%
8	7.559	723	727	733	rBV	12825	20430	1.25%	0.094%
9	7.964	789	796	804	rBV	250286	415753	25.44%	1.904%
10	8.657	906	914	924	rBV	236020	407167	24.91%	1.865%
11	9.116	985	992	1000	rBV	168737	289781	17.73%	1.327%
12	9.292	1016	1022	1026	rBV2	2162	3690	0.23%	0.017%
13	9.838	1108	1115	1122	rBV	119325	205108	12.55%	0.939%
14	10.055	1147	1152	1160	rBV4	3632	7612	0.47%	0.035%
15	10.373	1199	1206	1217	rBV	239715	420032	25.70%	1.923%
16	10.531	1229	1233	1238	rBV3	2705	4105	0.25%	0.019%
17	10.760	1262	1272	1279	rBV	373650	667402	40.83%	3.056%
18	10.884	1285	1293	1305	rBV	215696	382760	23.42%	1.753%
19	11.295	1357	1363	1370	rVB2	2558	4171	0.26%	0.019%
20	11.495	1391	1397	1403	rBV2	24785	45581	2.79%	0.209%
21	12.341	1536	1541	1547	rBV3	3606	5879	0.36%	0.027%
22	12.957	1641	1646	1651	rVB	4207	6048	0.37%	0.028%
23	13.204	1683	1688	1691	rBV4	4468	7191	0.44%	0.033%
24	13.427	1721	1726	1731	rBV3	3215	5150	0.32%	0.024%
25	13.903	1804	1807	1814	rVB2	6455	9687	0.59%	0.044%
26	13.991	1814	1822	1828	rBV	449274	643446	39.37%	2.947%
27	14.273	1858	1870	1880	rVB2	519176	819439	50.13%	3.752%
28	14.502	1905	1909	1914	rVV	2649	3837	0.23%	0.018%
29	14.585	1914	1923	1931	rVV	702142	1076374	65.85%	4.929%
30	14.755	1945	1952	1956	rBV	158360	260729	15.95%	1.194%
31	14.796	1956	1959	1960	rBV2	45668	47733	2.92%	0.219%
32	15.008	1989	1995	1997	rBV3	2461	3752	0.23%	0.017%
33	15.096	2006	2010	2012	rBV3	2530	3412	0.21%	0.016%
34	15.401	2057	2062	2066	rBV	6549	9757	0.60%	0.045%
35	15.454	2066	2071	2077	rVV2	4126	4442	0.27%	0.020%
36	15.572	2085	2091	2100	rBV	729329	1123297	68.72%	5.144%

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37	15.677	2104	2109	2115	rVV	101207	146545	8.97%	0.671%
38	15.812	2129	2132	2138	rBV4	2555	3846	0.24%	0.018%
39	16.130	2182	2186	2193	rVB4	12160	17794	1.09%	0.081%
40	16.318	2214	2218	2220	rVV3	4444	6258	0.38%	0.029%
41	16.488	2242	2247	2251	rBV4	2572	4144	0.25%	0.019%
42	16.723	2284	2287	2292	rBV3	2535	4118	0.25%	0.019%
43	17.111	2348	2353	2356	rBV3	6763	8138	0.50%	0.037%
44	17.263	2373	2379	2382	rBV3	4690	5693	0.35%	0.026%
45	17.322	2382	2389	2395	rVV	842856	1303941	79.77%	5.971%
46	17.422	2399	2406	2415	rVV	771359	1163130	71.16%	5.326%
47	17.504	2418	2420	2425	rVV5	2750	4064	0.25%	0.019%
48	17.622	2435	2440	2442	rBV3	3184	3712	0.23%	0.017%
49	17.716	2453	2456	2462	rVB5	5459	8694	0.53%	0.040%
50	17.845	2475	2478	2482	rVB4	4895	6649	0.41%	0.030%
51	18.015	2501	2507	2511	rVB2	23897	31955	1.95%	0.146%
52	18.233	2537	2544	2553	rBV	121519	206956	12.66%	0.948%
53	18.538	2592	2596	2600	rVV4	9614	11641	0.71%	0.053%
54	18.697	2619	2623	2625	rBV4	5447	6336	0.39%	0.029%
55	19.032	2678	2680	2683	rVV3	3761	4667	0.29%	0.021%
56	19.096	2686	2691	2700	rVV6	28399	56163	3.44%	0.257%
57	19.173	2700	2704	2707	rVB2	13326	18733	1.15%	0.086%
58	19.267	2717	2720	2724	rVB5	11587	15353	0.94%	0.070%
59	19.337	2726	2732	2735	rBV2	12645	25279	1.55%	0.116%
60	19.372	2735	2738	2744	rVB	21050	30685	1.88%	0.141%
61	19.437	2746	2749	2753	rVB6	6431	7858	0.48%	0.036%
62	19.501	2755	2760	2771	rBV2	49381	91717	5.61%	0.420%
63	19.660	2783	2787	2788	rBV4	6882	7612	0.47%	0.035%
64	19.701	2788	2794	2805	rVB	998605	1473711	90.16%	6.749%
65	19.848	2817	2819	2822	rVB4	5882	4971	0.30%	0.023%
66	19.913	2828	2830	2835	rBV6	3905	5322	0.33%	0.024%
67	20.236	2881	2885	2888	rBV2	31929	40046	2.45%	0.183%
68	20.277	2889	2892	2895	rVB2	20356	20874	1.28%	0.096%
69	20.588	2943	2945	2950	rVB5	5454	4997	0.31%	0.023%
70	20.700	2961	2964	2966	rBV4	8252	9369	0.57%	0.043%
71	20.741	2969	2971	2974	rVV3	10834	13795	0.84%	0.063%
72	20.770	2974	2976	2981	rVB2	16737	16110	0.99%	0.074%
73	21.082	3026	3029	3034	rBV6	8731	12839	0.79%	0.059%
74	21.252	3052	3058	3072	rBV	479996	724208	44.31%	3.316%
75	21.563	3104	3111	3117	rBV	876344	1440876	88.15%	6.598%
76	21.804	3148	3152	3162	rBV2	38126	74391	4.55%	0.341%

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77	22.415	3249	3256	3267	rBV	288514	553935	33.89%	2.537%
78	22.838	3326	3328	3329	rBV	5291	4152	0.25%	0.019%
79	22.873	3330	3334	3339	rVB7	13240	24191	1.48%	0.111%
80	23.085	3366	3370	3385	rVB4	29555	76114	4.66%	0.349%
81	23.878	3498	3505	3509	rBV	87877	194102	11.87%	0.889%
82	24.048	3532	3534	3535	rBV2	5252	4471	0.27%	0.020%
83	24.454	3592	3603	3621	rVB	564275	1515732	92.73%	6.941%
84	24.665	3628	3639	3646	rBV	561289	1588522	97.18%	7.274%
85	24.730	3646	3650	3658	rVV	147112	367940	22.51%	1.685%
86	24.806	3658	3663	3670	rVB2	37569	84950	5.20%	0.389%
87	25.523	3782	3785	3786	rBV3	6912	7772	0.48%	0.036%
88	25.916	3842	3852	3860	rBV4	49770	155201	9.49%	0.711%
89	26.010	3862	3868	3881	rVB6	31435	103142	6.31%	0.472%
90	26.756	3993	3995	4000	rBV6	3971	5832	0.36%	0.027%
91	27.244	4070	4078	4085	rBV3	24337	71963	4.40%	0.330%
92	28.824	4344	4347	4348	rBV3	7360	7598	0.46%	0.035%
93	29.664	4480	4490	4491	rBV9	12672	29831	1.83%	0.137%
94	29.846	4508	4521	4535	rBV9	50353	219867	13.45%	1.007%
95	30.117	4557	4567	4571	rBV9	14474	40599	2.48%	0.186%
96	30.616	4641	4652	4653	rBV9	22968	51094	3.13%	0.234%
97	30.786	4672	4681	4683	rVV9	12295	30989	1.90%	0.142%
98	31.256	4754	4761	4762	rBV6	17369	32054	1.96%	0.147%
99	31.891	4846	4869	4890	rBV7	281097	1634560	100.00%	7.485%
100	32.525	4967	4977	4979	rBV10	9496	26086	1.60%	0.119%

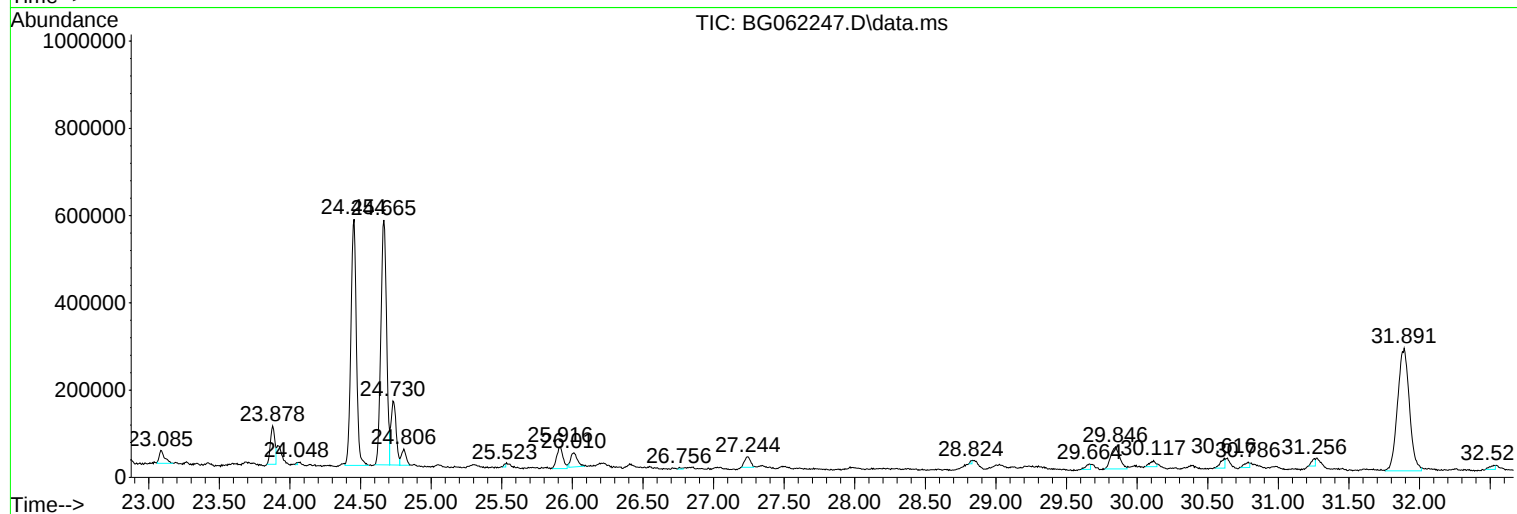
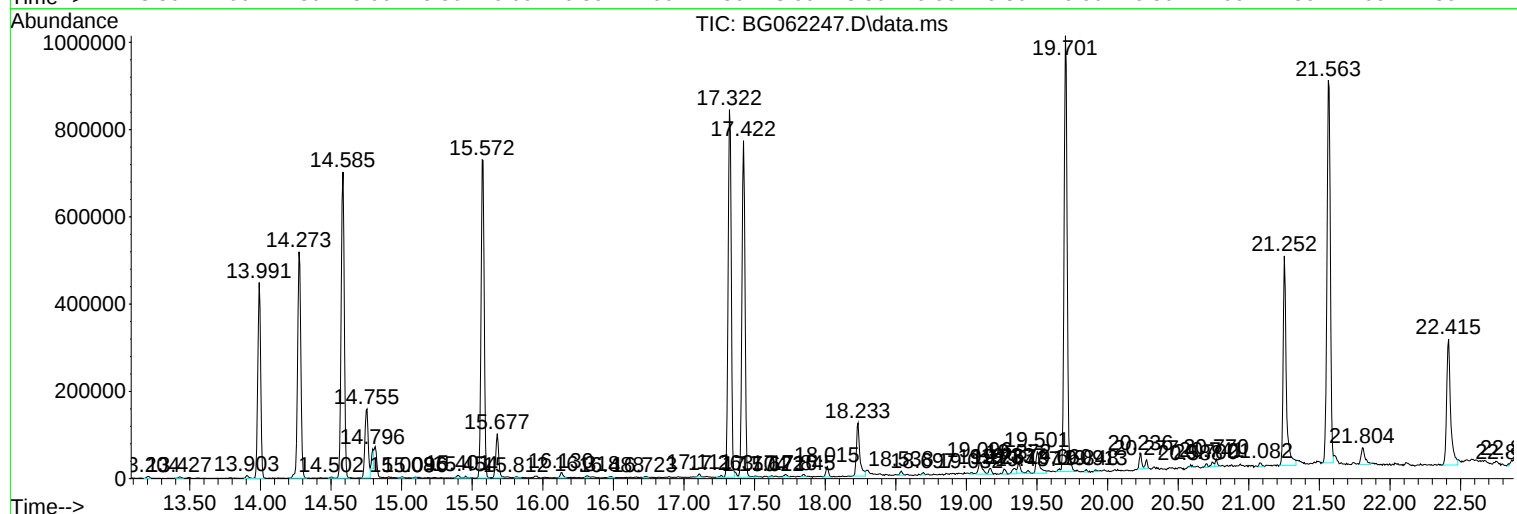
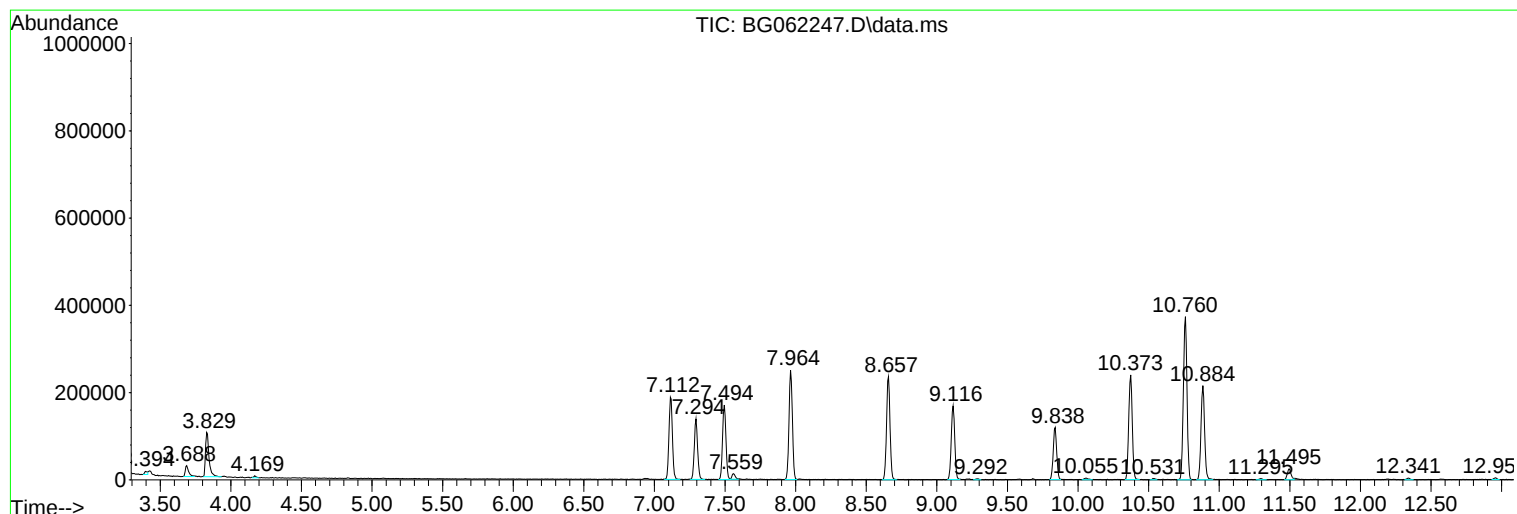
Sum of corrected areas: 21837193

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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



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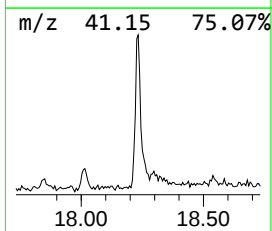
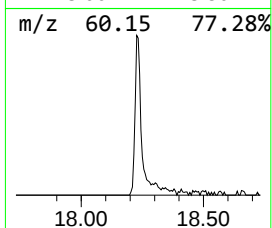
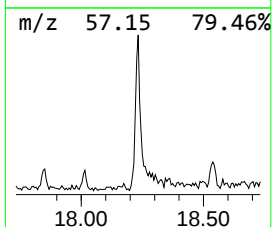
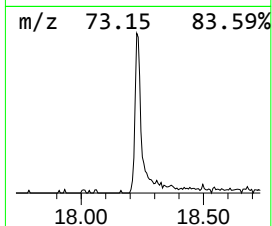
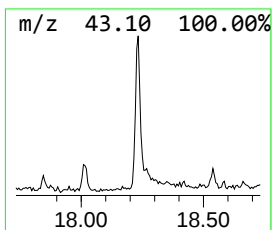
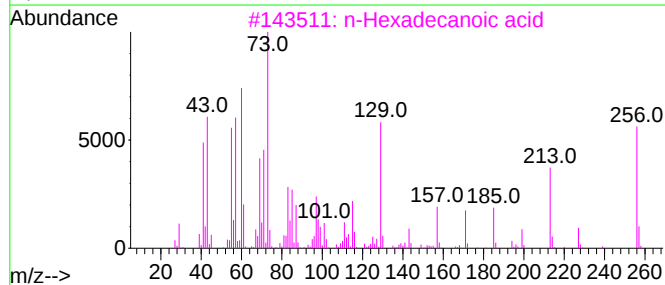
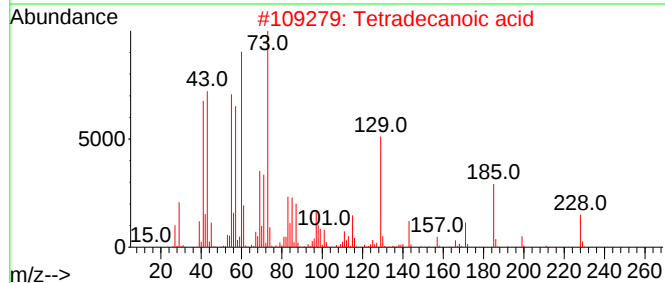
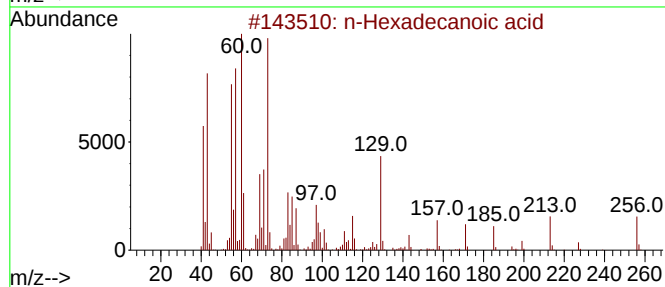
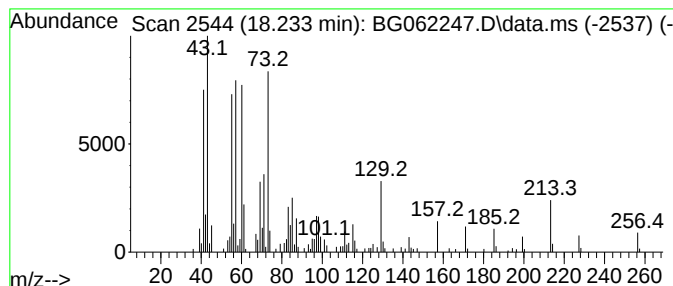
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	3.17 ng/ul	206956	Phenanthrene-d10	17.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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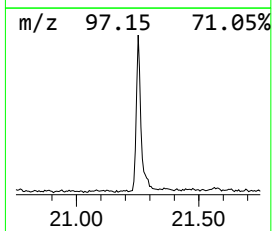
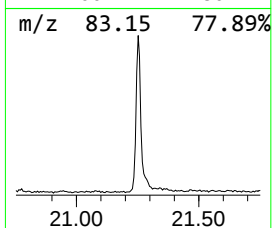
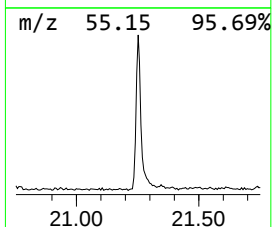
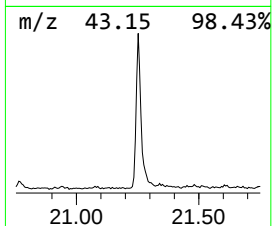
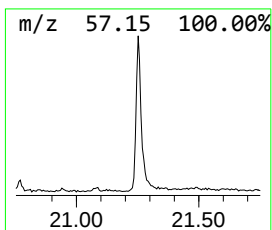
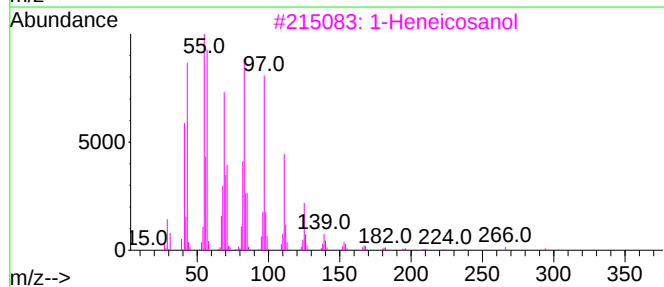
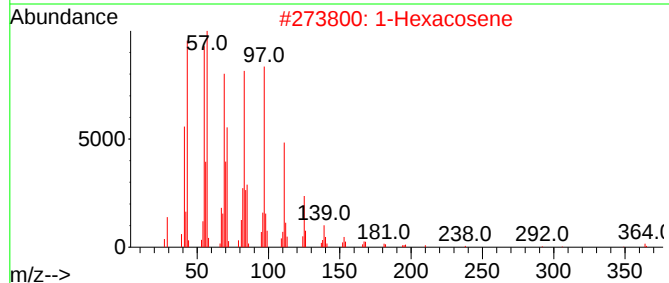
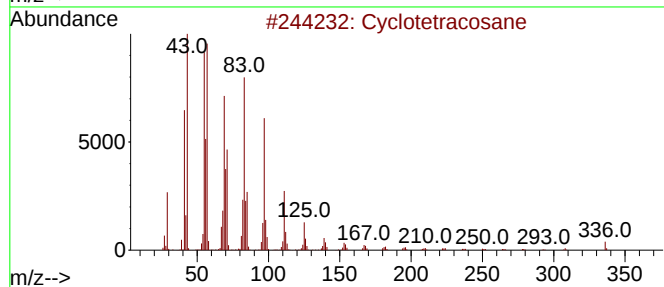
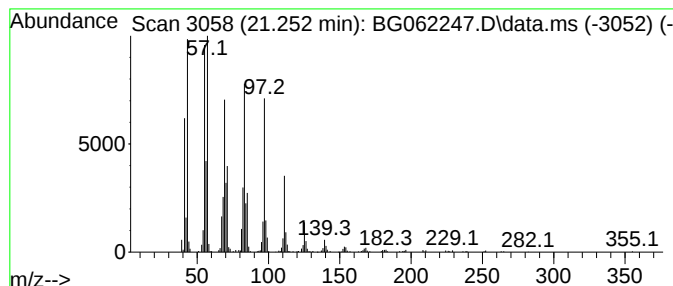
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TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic21.252 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.252	10.05 ng/ul	724208	Chrysene-d12	21.569

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	94
2		1-Hexacosene	364	C26H52	018835-33-1	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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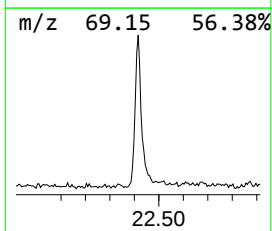
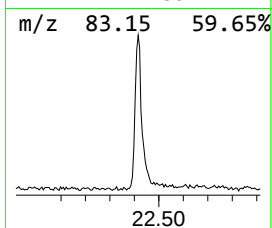
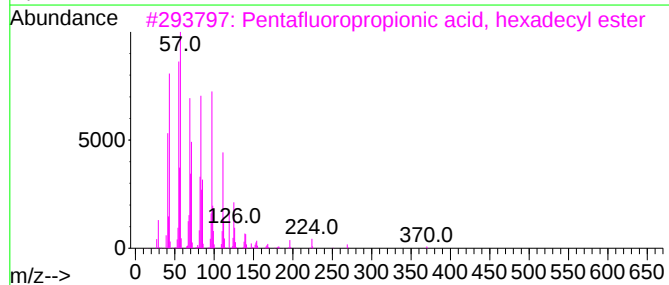
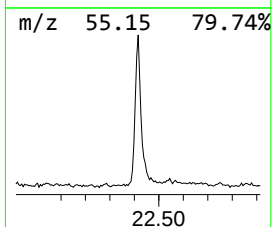
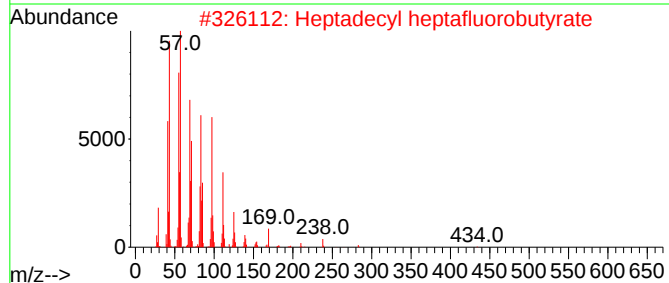
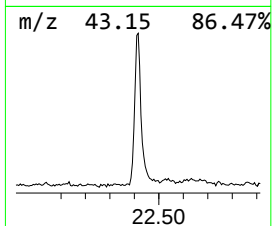
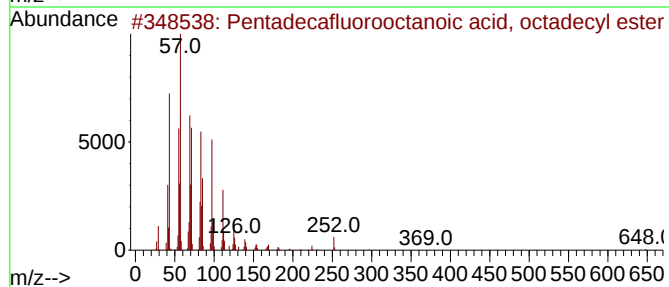
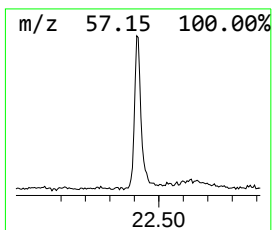
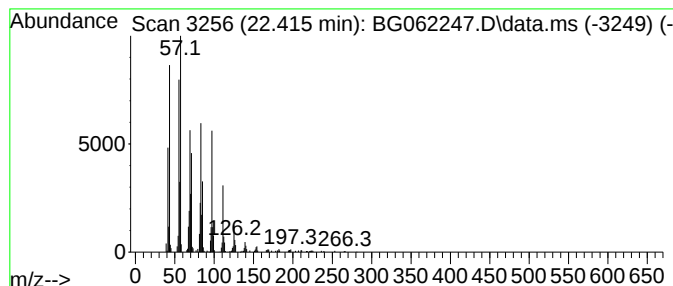
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.415	7.69 ng/ul	553935	Chrysene-d12	21.569	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
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Acq On : 5 Aug 2024 21:27
Operator : MA/JU
Sample : P3361-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

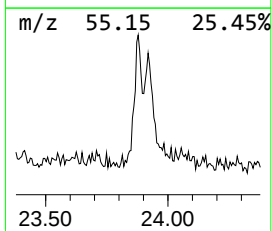
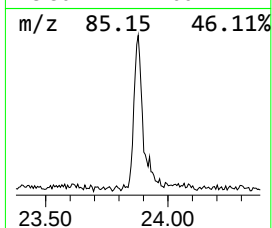
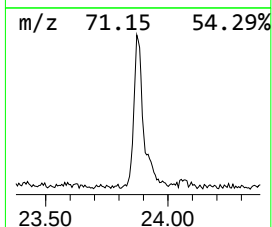
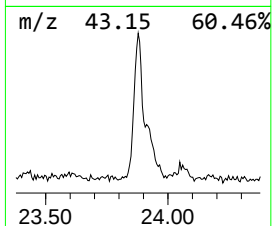
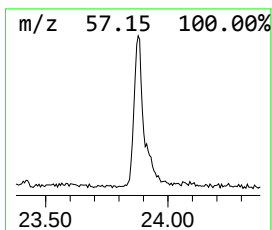
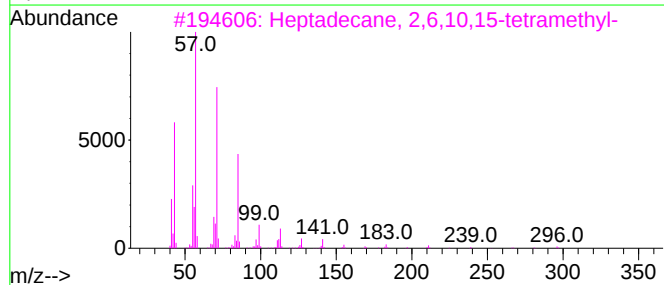
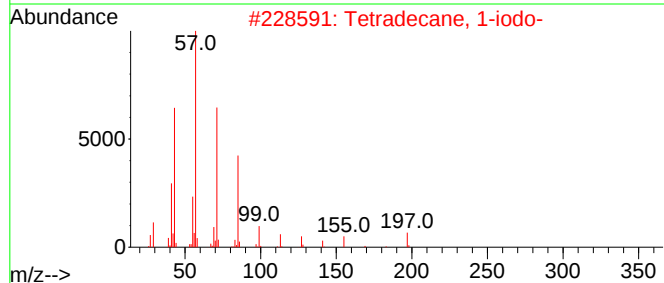
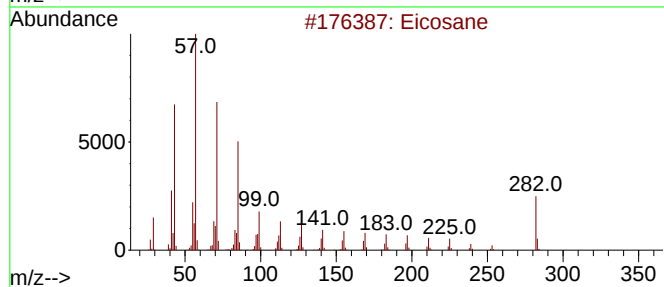
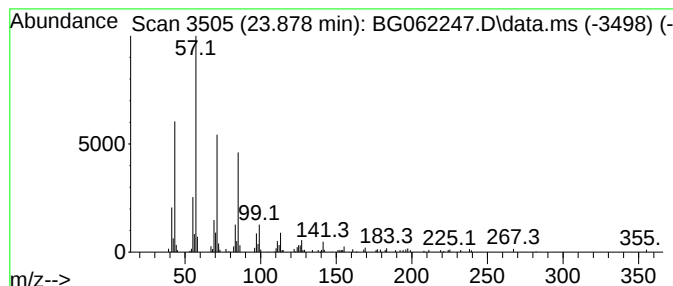
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.878	2.44 ng/ul	194102	Perylene-d12		24.665	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	91
3	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062247.D
Acq On : 5 Aug 2024 21:27
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Sample : P3361-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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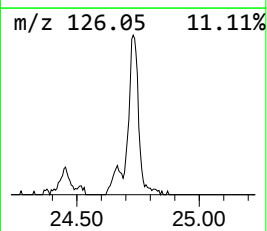
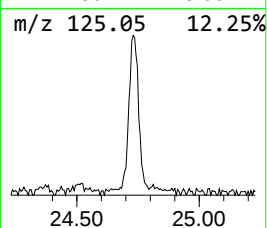
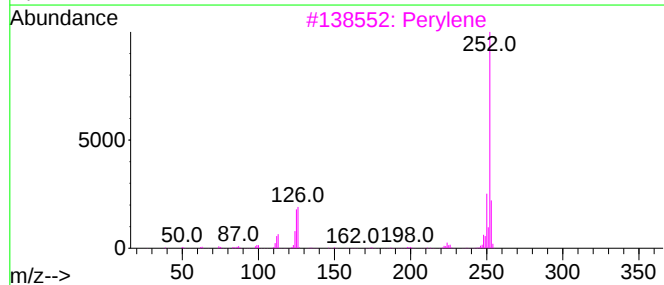
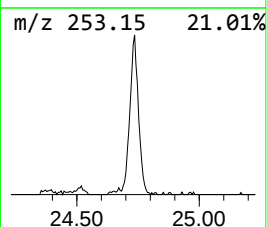
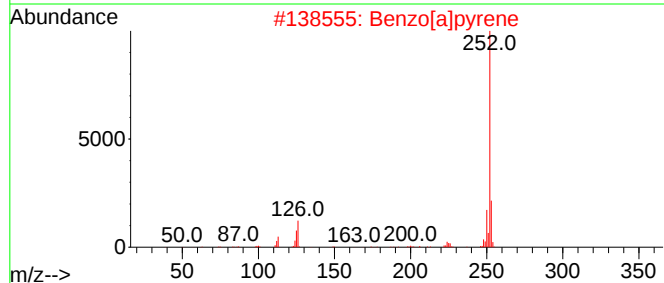
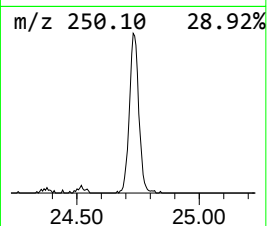
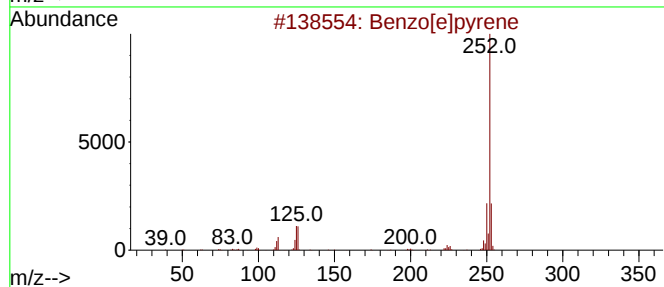
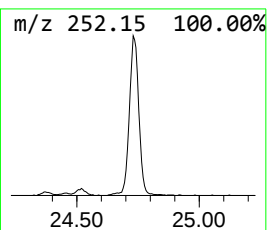
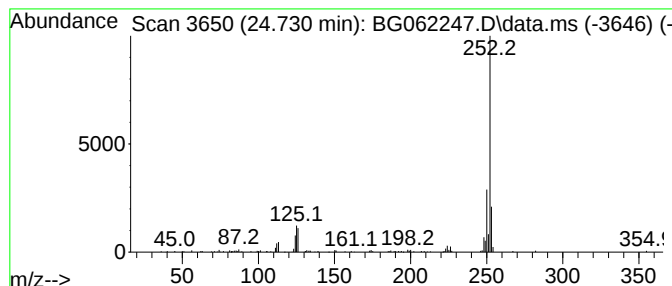
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.730	4.63 ng/ul	367940	Perylene-d12	24.665

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Perylene	252	C20H12	000198-55-0	91
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062247.D
Acq On : 5 Aug 2024 21:27
Operator : MA/JU
Sample : P3361-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P0

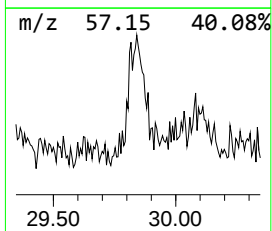
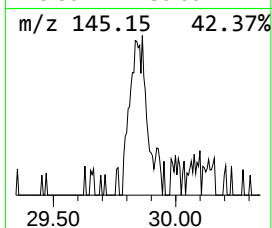
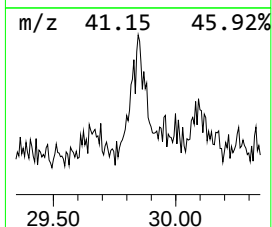
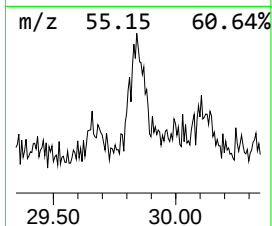
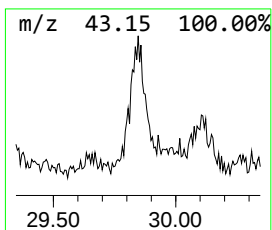
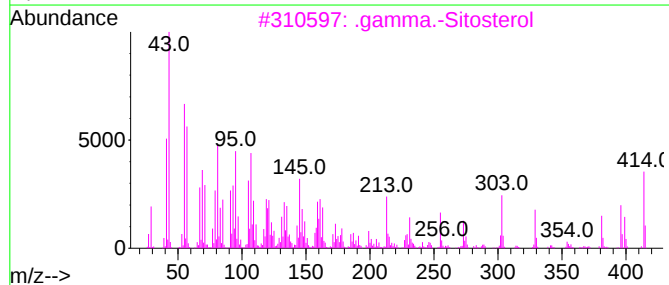
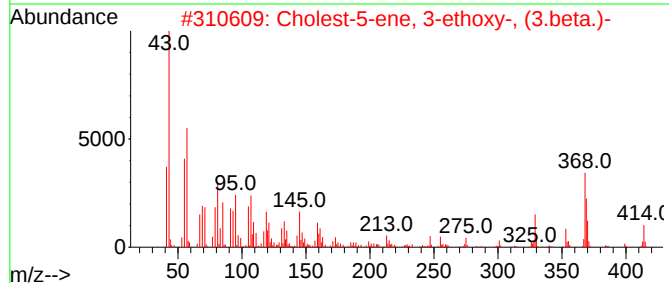
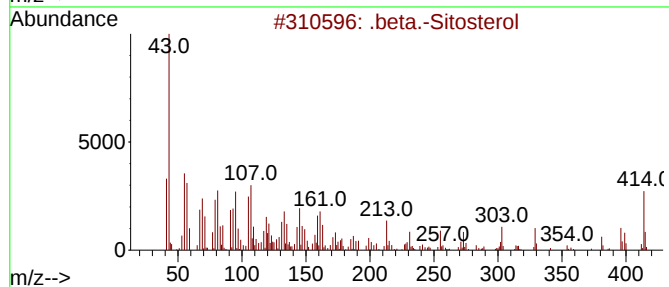
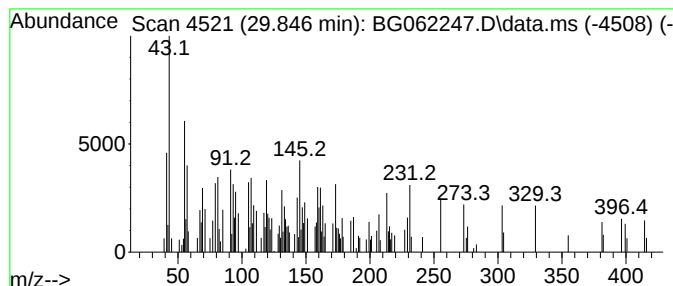
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.846	2.77 ng/ul	219867	Perylene-d12	24.665

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	50
2			Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	38
3			.gamma.-Sitosterol	414	C29H50O	000083-47-6	35
4			.beta.-Sitosterol	414	C29H50O	000083-46-5	35
5			Stigmasta-3,5-diene	396	C29H48	004970-37-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062247.D
Acq On : 5 Aug 2024 21:27
Operator : MA/JU
Sample : P3361-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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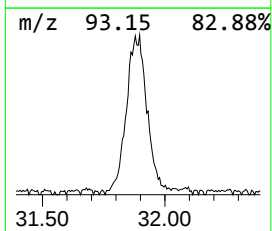
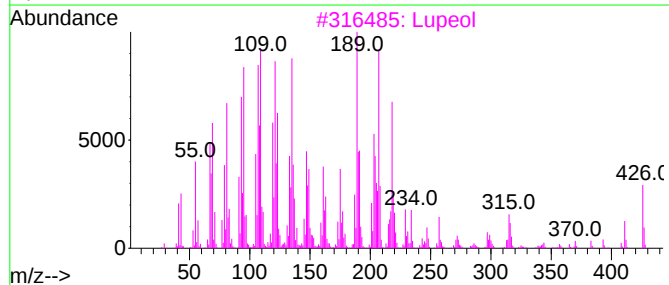
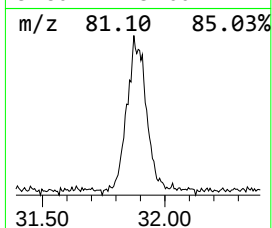
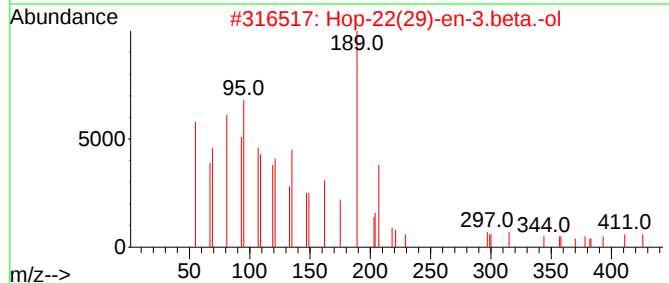
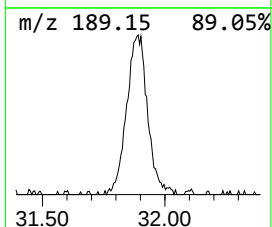
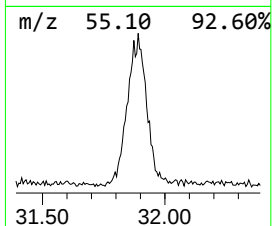
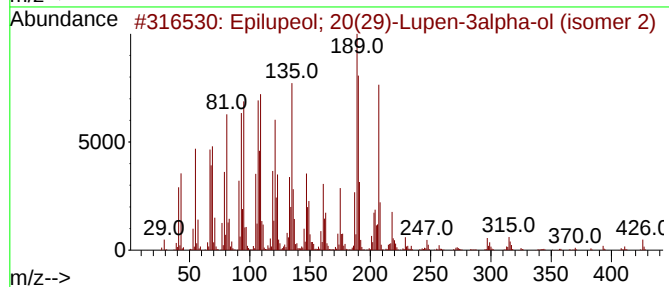
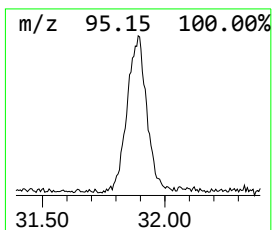
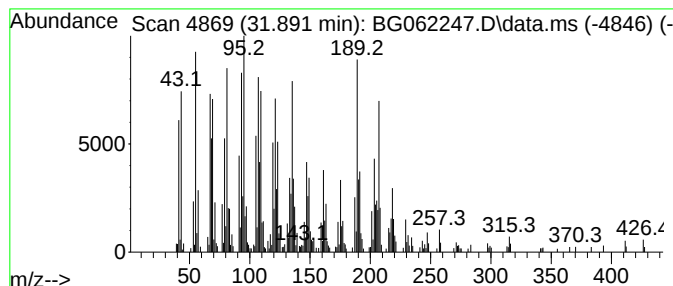
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Epilupeol; 20(29)-Lupen-3al... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.891	20.58 ng/ul	1634560	Perylene-d12	24.665

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	95
2			Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	93
3			Lupeol	426	C30H50O	000545-47-1	90
4			Lupeol	426	C30H50O	000545-47-1	90
5			Taraxasterol	426	C30H50O	001059-14-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
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Acq On : 5 Aug 2024 21:27
Operator : MA/JU
Sample : P3361-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
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
n-Hexadecanoic ...	18.233	3.2	ng/ul	206956	4	17.322	1303940	20.0
(DEL) Alkane: C...	21.252	10.1	ng/ul	724208	5	21.569	1440880	20.0
Pentadecafluoro...	22.415	7.7	ng/ul	553935	5	21.569	1440880	20.0
(DEL) Alkane: S...	23.878	2.4	ng/ul	194102	6	24.665	1588520	20.0
Benzo[e]pyrene	24.730	4.6	ng/ul	367940	6	24.665	1588520	20.0
.beta.-Sitosterol	29.846	2.8	ng/ul	219867	6	24.665	1588520	20.0
Epilupeol; 20(2...	31.891	20.6	ng/ul	1634560	6	24.665	1588520	20.0