

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
 Data File : BP013301.D
 Acq On : 24 Dec 2022 15:49
 Operator : CG/JU
 Sample : N6016-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBYD2

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_P\Methods\SFAM-EPA-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP013301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	21	25	33	rVB	114089	157105	1.54%	0.117%
2	3.758	94	97	111	rBV	1335449	1998100	19.52%	1.494%
3	3.864	111	115	122	rVV	147315	202067	1.97%	0.151%
4	3.940	125	128	133	rVB2	22587	27332	0.27%	0.020%
5	4.087	149	153	163	rVB	47721	68107	0.67%	0.051%
6	4.317	188	192	198	rVB2	33314	47057	0.46%	0.035%
7	4.458	213	216	221	rVB6	13324	20745	0.20%	0.016%
8	4.652	246	249	253	rVB2	25798	32320	0.32%	0.024%
9	4.728	260	262	270	rVB7	14023	19967	0.20%	0.015%
10	5.034	308	314	322	rVB2	68296	112118	1.10%	0.084%
11	5.117	325	328	331	rVV	35293	47552	0.46%	0.036%
12	5.152	332	334	341	rVB4	23569	30816	0.30%	0.023%
13	5.264	350	353	360	rVB3	20844	35934	0.35%	0.027%
14	6.528	565	568	574	rVV6	11297	21050	0.21%	0.016%
15	6.611	577	582	589	rVB	159208	243290	2.38%	0.182%
16	6.922	630	635	638	rBV5	16622	25962	0.25%	0.019%
17	7.105	658	666	679	rBV	1829138	2946758	28.79%	2.203%
18	7.216	679	685	688	rBV	34653	50952	0.50%	0.038%
19	7.269	688	694	706	rVV	1486527	2314523	22.62%	1.730%
20	7.369	707	711	718	rVB	28637	50269	0.49%	0.038%
21	7.469	721	728	738	rBV	1931178	2965861	28.98%	2.217%
22	7.940	801	808	815	rBV	2435037	3708762	36.24%	2.772%
23	8.652	921	929	941	rBV	2153487	3394060	33.16%	2.537%
24	9.110	998	1007	1016	rBV	1674723	2779435	27.16%	2.078%
25	9.269	1029	1034	1041	rVB7	22308	39948	0.39%	0.030%
26	9.505	1066	1074	1086	rVB	58094	107568	1.05%	0.080%
27	9.834	1120	1130	1143	rBV	1391484	2342432	22.89%	1.751%
28	9.987	1152	1156	1163	rBV9	12296	26169	0.26%	0.020%
29	10.063	1163	1169	1175	rVB9	23367	45970	0.45%	0.034%
30	10.375	1212	1222	1233	rBV	2079996	3501438	34.21%	2.617%
31	10.752	1277	1286	1294	rBV	2922000	4931291	48.18%	3.686%
32	10.893	1302	1310	1326	rBV	1535513	2679007	26.18%	2.003%
33	11.222	1362	1366	1371	rVB8	12596	19273	0.19%	0.014%
34	11.281	1371	1376	1381	rBV9	15113	25483	0.25%	0.019%
35	12.163	1521	1526	1531	rBV2	25857	43805	0.43%	0.033%
36	12.240	1533	1539	1545	rBV4	13647	18674	0.18%	0.014%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
 Title : SVOA CALIBRATION

37	12.334	1545	1555	1561	rBV	38872	74695	0.73%	0.056%
38	12.740	1621	1624	1627	rVV4	13786	20301	0.20%	0.015%
39	12.787	1627	1632	1636	rVV8	10937	24096	0.24%	0.018%
40	12.851	1640	1643	1648	rVV7	12571	19610	0.19%	0.015%
41	12.969	1654	1663	1668	rVB10	11282	32610	0.32%	0.024%
42	13.104	1683	1686	1692	rVB6	14023	21641	0.21%	0.016%
43	13.322	1717	1723	1725	rBV7	22286	37327	0.36%	0.028%
44	13.398	1729	1736	1742	rVB2	54452	85954	0.84%	0.064%
45	13.451	1742	1745	1751	rBV6	41122	68583	0.67%	0.051%
46	13.904	1816	1822	1829	rBV	328825	463419	4.53%	0.346%
47	13.993	1829	1837	1845	rBV	3053145	4259584	41.62%	3.184%
48	14.051	1845	1847	1853	rVV7	22283	41621	0.41%	0.031%
49	14.104	1853	1856	1861	rVB6	22355	36144	0.35%	0.027%
50	14.281	1879	1886	1897	rVV	3442005	5150848	50.33%	3.850%
51	14.422	1905	1910	1913	rBV3	28788	40021	0.39%	0.030%
52	14.469	1915	1918	1922	rVB	35150	46443	0.45%	0.035%
53	14.540	1925	1930	1932	rBV	89987	118805	1.16%	0.089%
54	14.587	1932	1938	1945	rVV	3482427	5119023	50.02%	3.826%
55	14.645	1945	1948	1953	rVB2	53126	68483	0.67%	0.051%
56	14.787	1966	1972	1977	rBV	946297	1527630	14.93%	1.142%
57	14.940	1995	1998	2002	rVB5	20009	26299	0.26%	0.020%
58	14.987	2002	2006	2012	rVV8	29554	45860	0.45%	0.034%
59	15.040	2012	2015	2022	rVB9	18515	28516	0.28%	0.021%
60	15.110	2024	2027	2030	rVB5	14589	19127	0.19%	0.014%
61	15.310	2058	2061	2066	rVB6	14824	19474	0.19%	0.015%
62	15.422	2078	2080	2084	rVB5	19329	19174	0.19%	0.014%
63	15.492	2084	2092	2098	rBV2	169028	253284	2.47%	0.189%
64	15.581	2100	2107	2114	rBV	4222388	6016673	58.79%	4.497%
65	15.698	2121	2127	2137	rBV	830209	1134604	11.09%	0.848%
66	15.822	2144	2148	2155	rVB4	29743	52877	0.52%	0.040%
67	15.945	2165	2169	2175	rVB	52412	82537	0.81%	0.062%
68	16.045	2179	2186	2195	rVB6	67491	181431	1.77%	0.136%
69	16.151	2199	2204	2210	rBV3	101814	155526	1.52%	0.116%
70	16.728	2298	2302	2307	rBV4	42410	62268	0.61%	0.047%
71	16.839	2318	2321	2329	rVB5	40744	51272	0.50%	0.038%
72	17.134	2367	2371	2375	rBV6	19663	35049	0.34%	0.026%
73	17.345	2401	2407	2417	rBV	3872509	5772760	56.41%	4.315%
74	17.445	2417	2424	2432	rVB	3953232	5786917	56.54%	4.326%
75	17.610	2448	2452	2460	rBV7	50242	88776	0.87%	0.066%
76	17.698	2464	2467	2469	rBV4	31636	38039	0.37%	0.028%

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77	18.157	2542	2545	2550	rVB5	83095	117778	1.15%	0.088%
78	18.216	2550	2555	2566	rBV	976225	1493579	14.59%	1.116%
79	18.410	2583	2588	2594	rVB	738925	946855	9.25%	0.708%
80	18.463	2594	2597	2601	rVB	74491	84127	0.82%	0.063%
81	18.551	2608	2612	2616	rBV2	74177	116292	1.14%	0.087%
82	18.628	2620	2625	2629	rBV	425999	559095	5.46%	0.418%
83	18.722	2638	2641	2647	rVB2	126401	172720	1.69%	0.129%
84	18.781	2647	2651	2658	rVB	317170	410929	4.02%	0.307%
85	19.122	2705	2709	2713	rBV	232077	278793	2.72%	0.208%
86	19.333	2738	2745	2747	rBV3	204163	405271	3.96%	0.303%
87	19.445	2760	2764	2773	rVB	318623	441126	4.31%	0.330%
88	19.675	2798	2803	2812	rBV	6114461	8155531	79.69%	6.096%
89	19.745	2812	2815	2821	rVB3	152552	187222	1.83%	0.140%
90	19.828	2825	2829	2836	rBV	906779	1255850	12.27%	0.939%
91	20.175	2884	2888	2893	rBV5	242559	536076	5.24%	0.401%
92	20.975	3021	3024	3029	rBV	653927	766028	7.48%	0.573%
93	21.127	3046	3050	3059	rBV	1731583	2338038	22.84%	1.748%
94	21.433	3097	3102	3113	rVB	5482561	7271933	71.05%	5.436%
95	23.127	3386	3390	3396	rVB	1447358	2223756	21.73%	1.662%
96	23.757	3490	3497	3511	rVB2	4743464	10234426	100.00%	7.650%
97	23.916	3518	3524	3533	rVB2	3790265	7663080	74.88%	5.728%
98	24.533	3623	3629	3638	rVB	3410234	7256810	70.91%	5.424%
99	24.639	3641	3647	3659	rVB2	1214490	3369512	32.92%	2.519%
100	26.445	3948	3954	3969	rVB	1687669	5288930	51.68%	3.953%

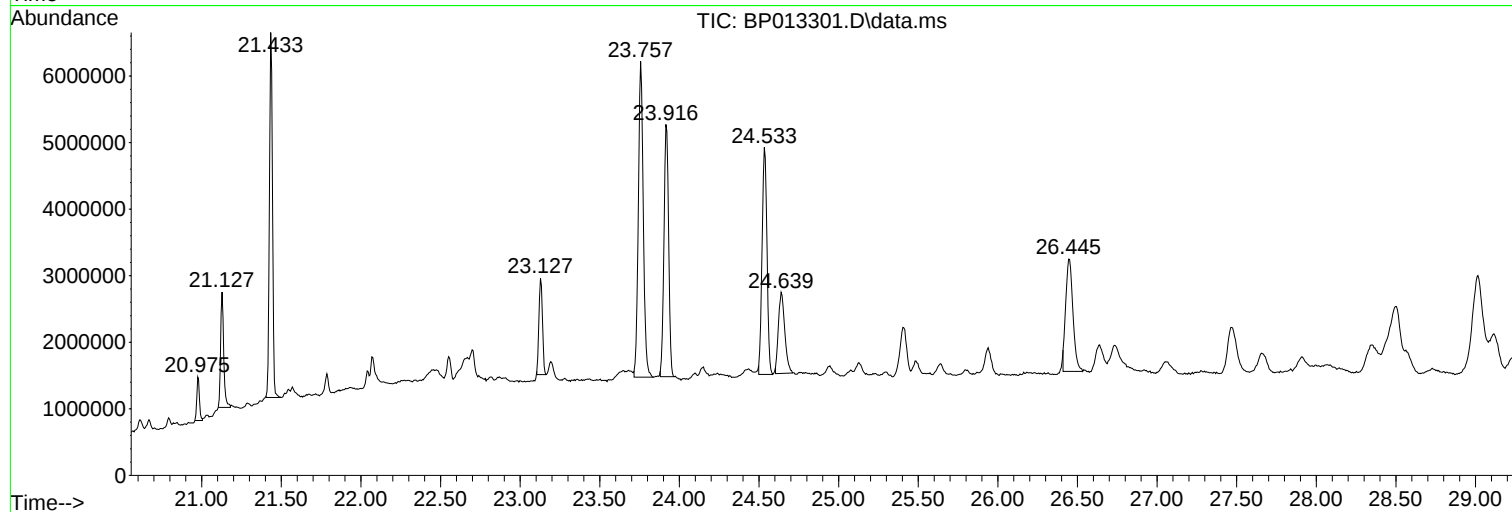
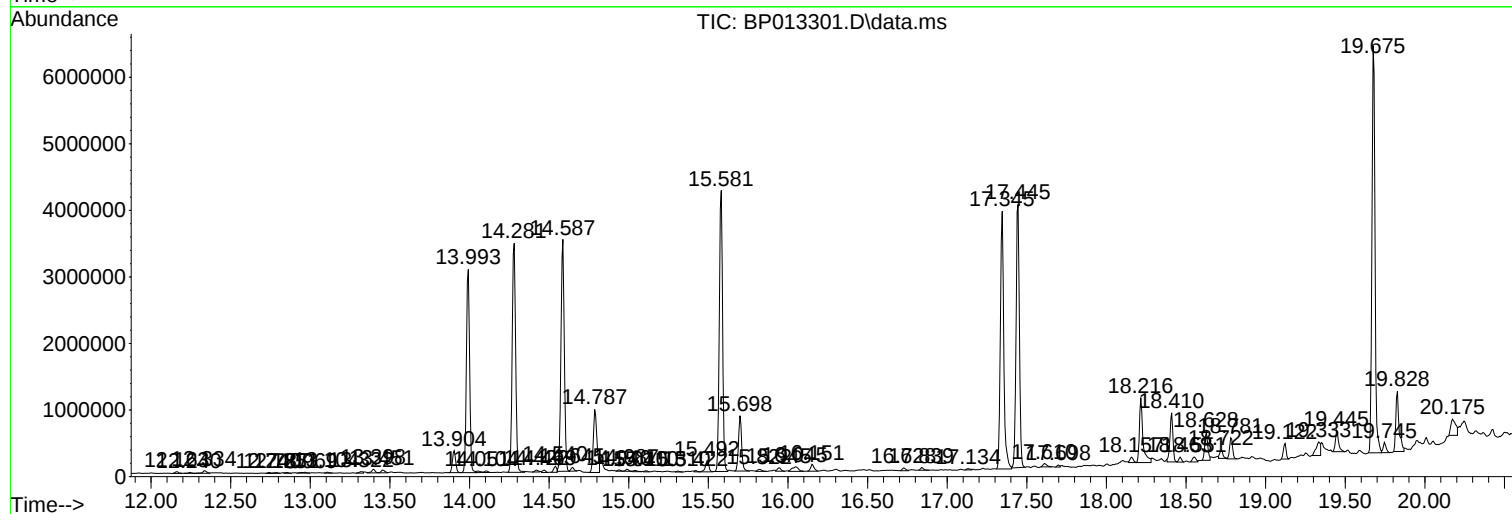
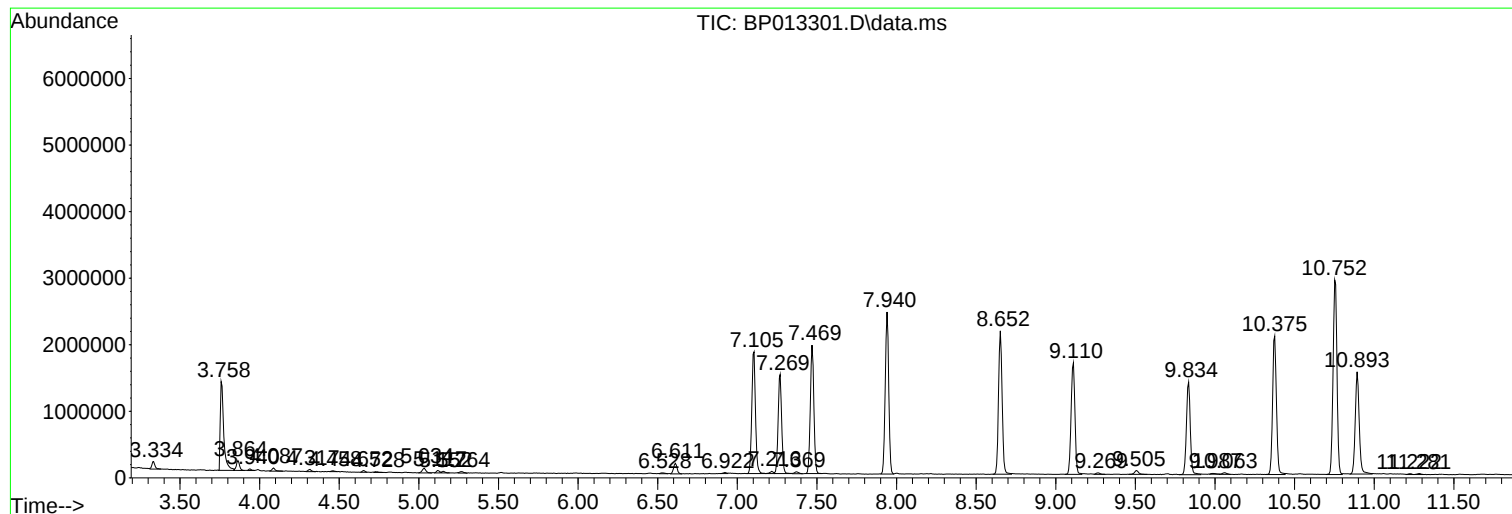
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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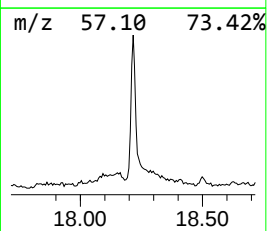
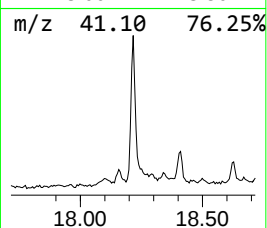
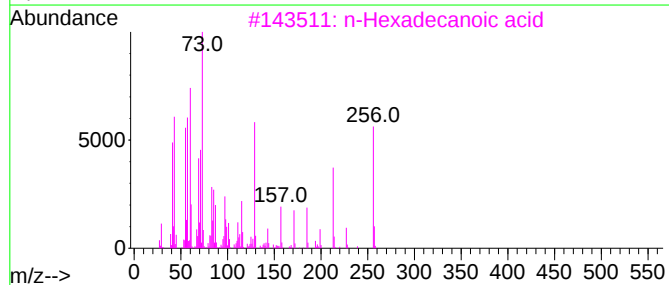
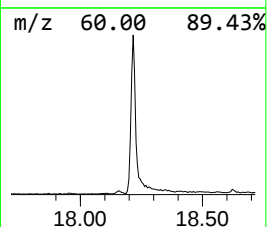
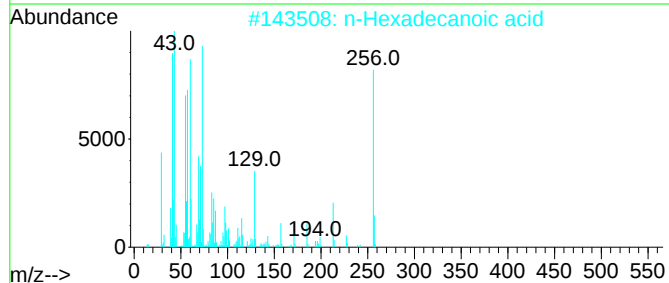
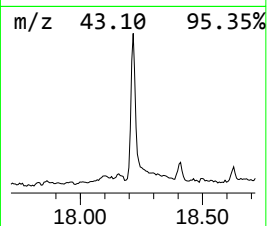
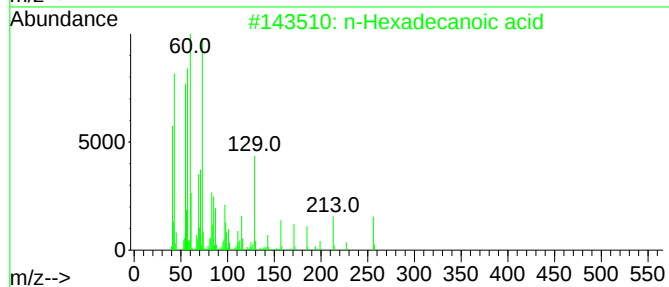
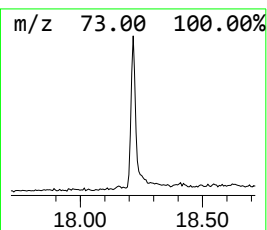
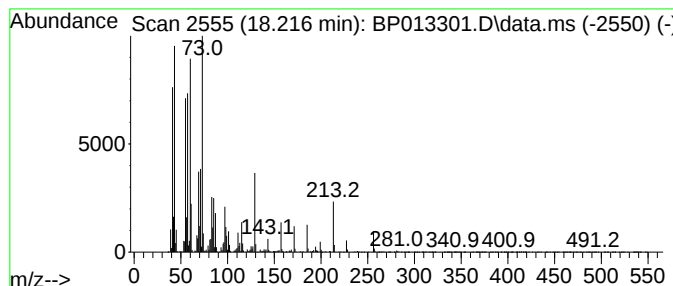
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	5.17 ng/ul	1493580	Phenanthrene-d10	17.345

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	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	93



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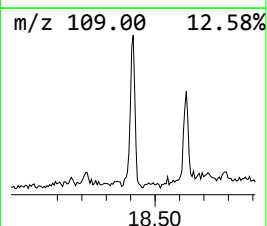
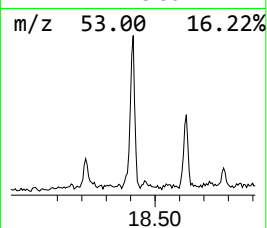
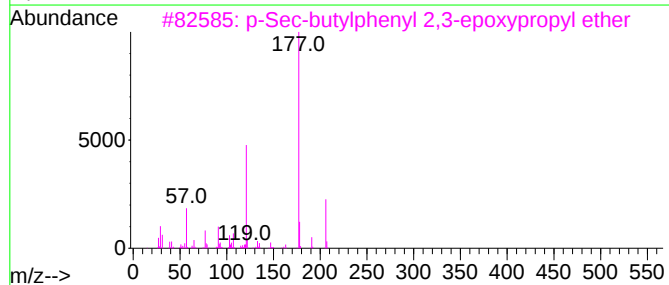
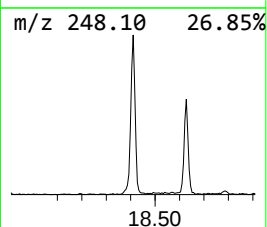
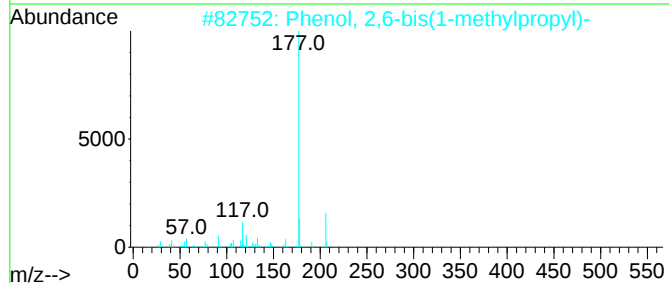
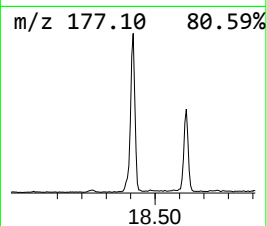
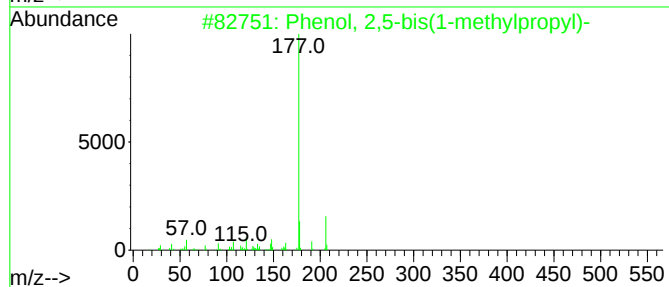
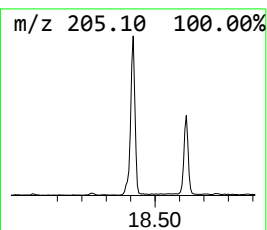
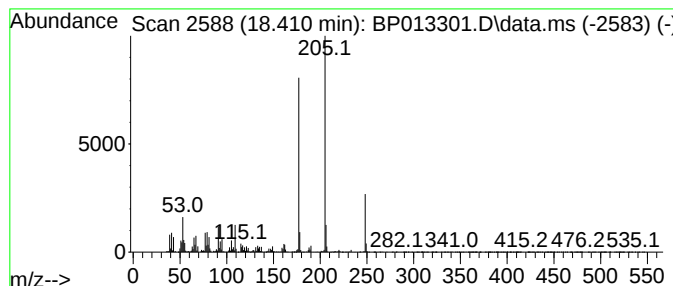
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.410	3.28 ng/ul	946855	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,5-bis(1-methylpropyl)-	206	C14H22O	054932-77-3	38
2			Phenol, 2,6-bis(1-methylpropyl)-	206	C14H22O	005510-99-6	38
3			p-Sec-butylphenyl 2,3-epoxypropyl...	206	C13H18O2	067557-76-0	38
4			Spiro[cyclopenta[d]-1,3,2-dioxab...	206	C12H19BO2	062238-26-0	35
5			2-Amino-4-hydroxy-6,7,8-trimethy...	205	C9H11N5O	013045-86-8	27



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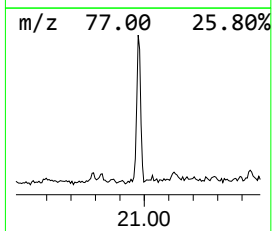
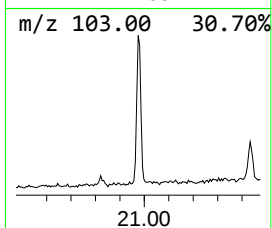
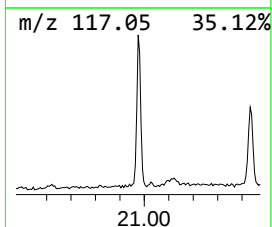
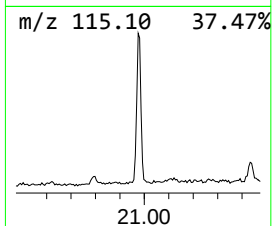
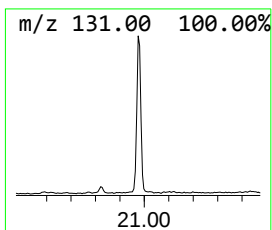
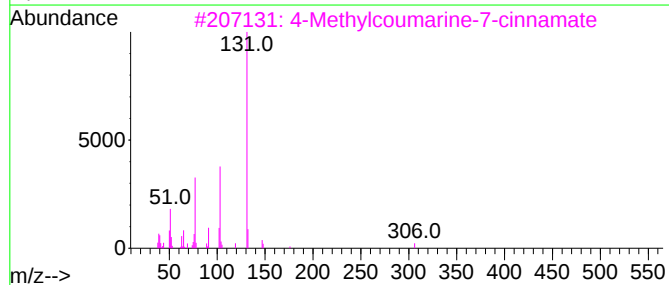
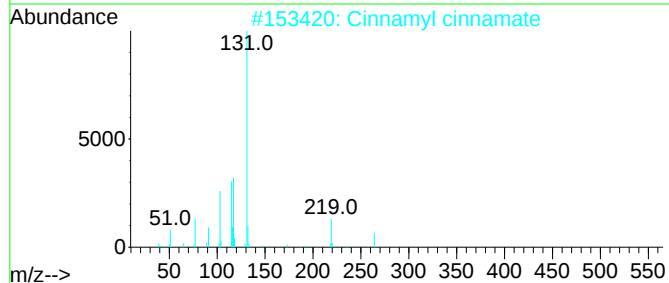
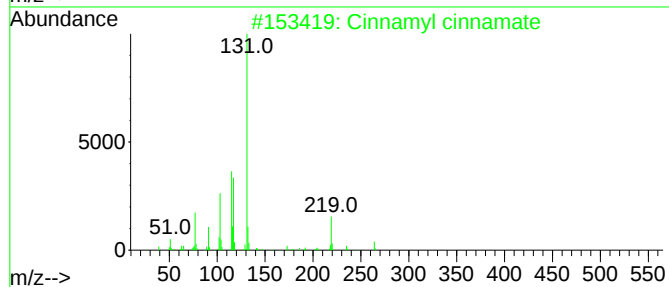
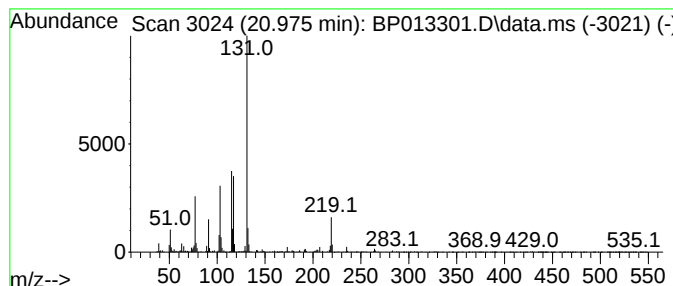
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Cinnamyl cinnamate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	2.11 ng/ul	766028	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	90
2			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	86
3			4-Methylcoumarine-7-cinnamate	306	C19H14O4	300829-05-4	64
4			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
5			3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013301.D
Acq On : 24 Dec 2022 15:49
Operator : CG/JU
Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD2

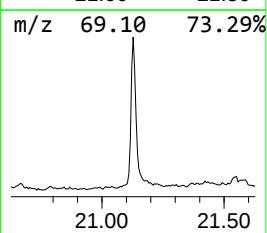
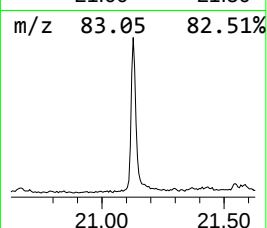
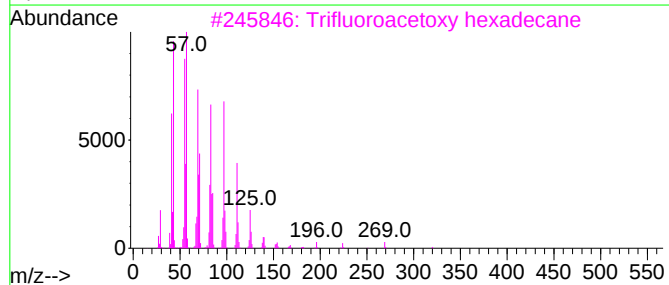
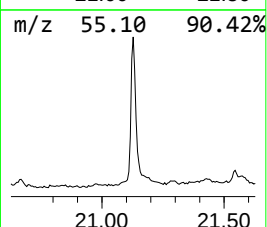
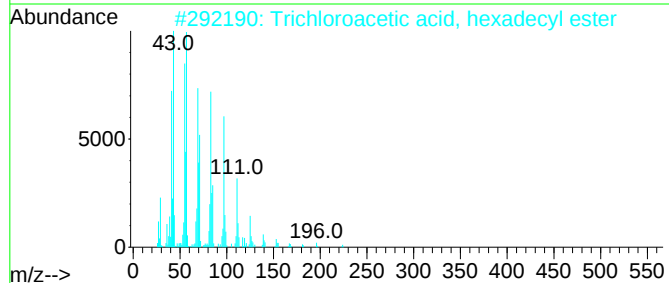
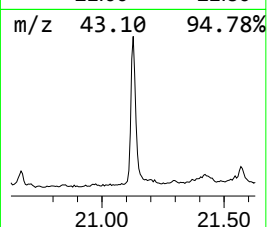
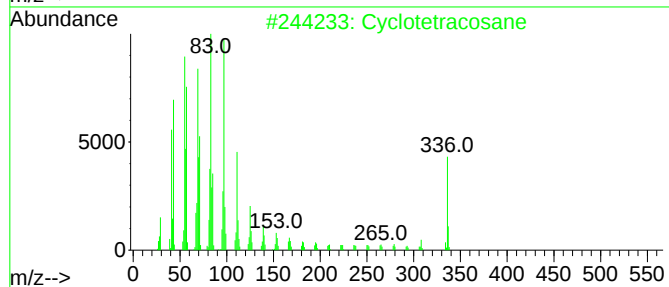
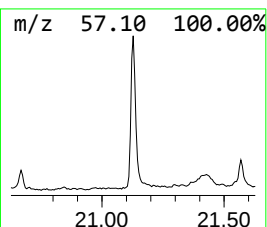
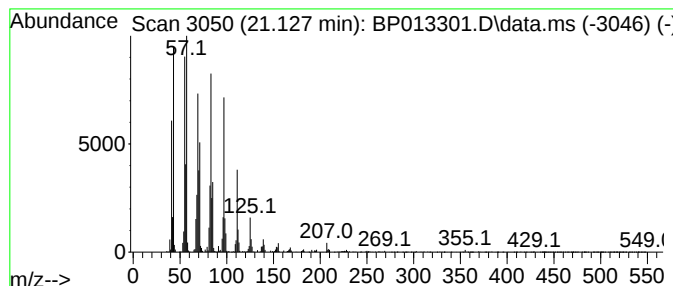
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Cyclic21.128 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	6.43 ng/ul	2338040	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	97
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013301.D
Acq On : 24 Dec 2022 15:49
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Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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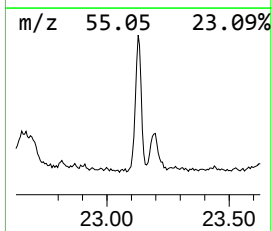
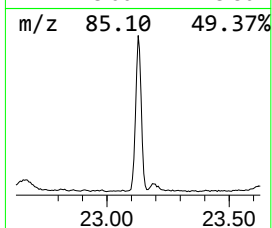
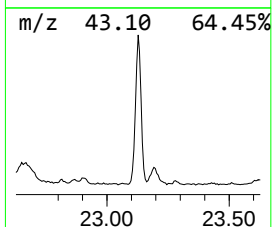
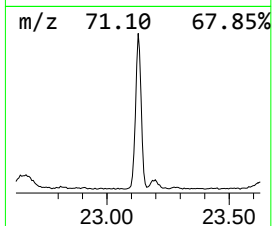
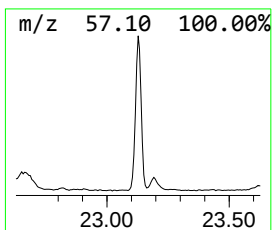
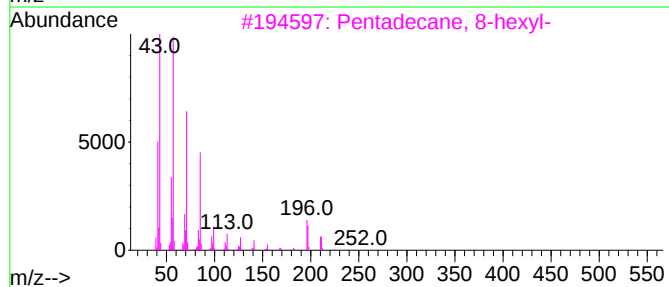
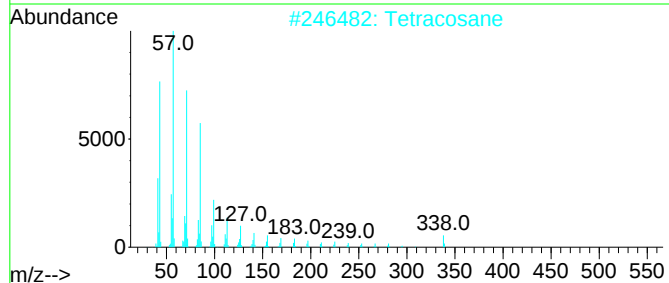
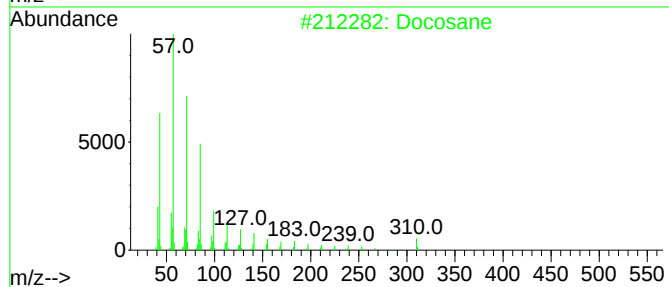
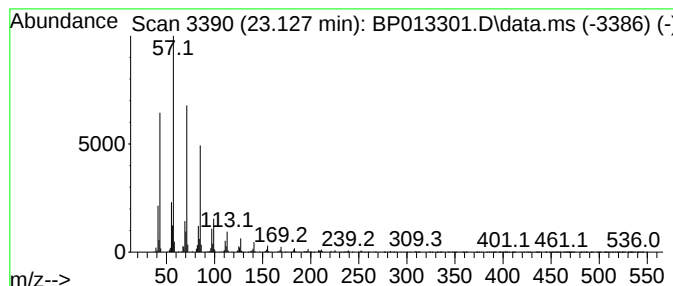
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	5.80 ng/ul	2223760	Perylene-d12	23.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	96
2			Tetracosane	338	C24H50	000646-31-1	96
3			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4			Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
5			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
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Acq On : 24 Dec 2022 15:49
Operator : CG/JU
Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

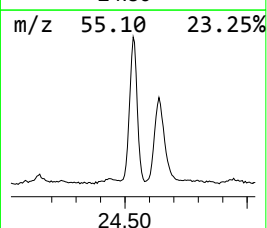
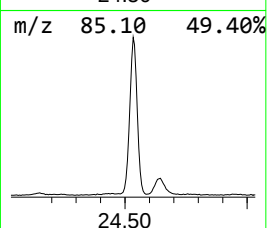
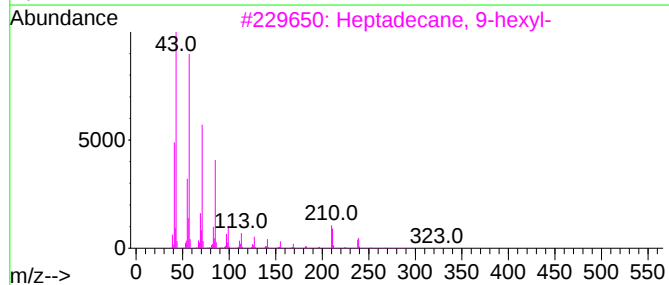
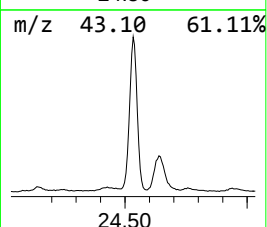
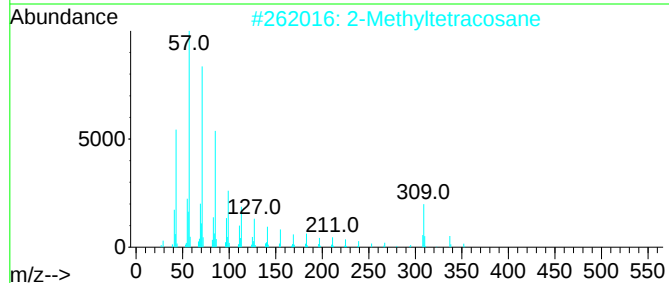
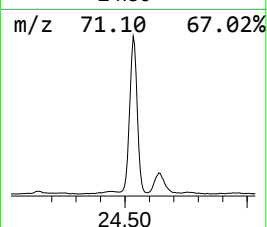
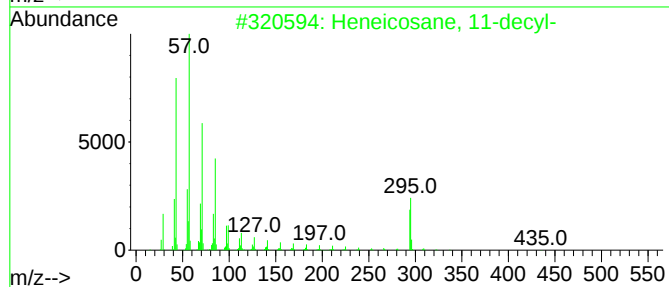
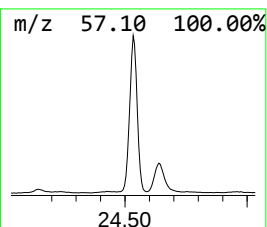
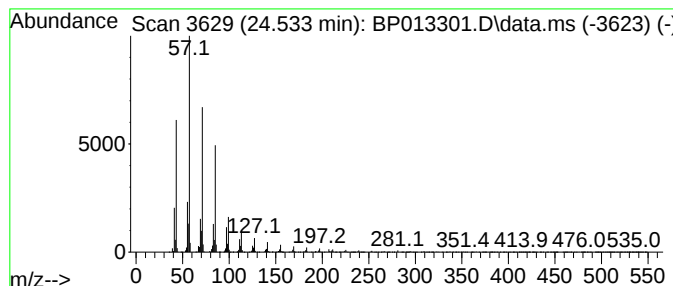
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.533	18.94 ng/ul	7256810	Perylene-d12	23.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	95
2	2-Methyltetracosane	352	C25H52	001560-78-7	94
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
4	Octacosane	394	C28H58	000630-02-4	93
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013301.D
Acq On : 24 Dec 2022 15:49
Operator : CG/JU
Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD2

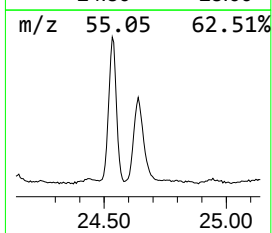
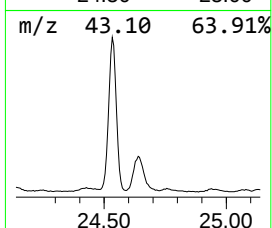
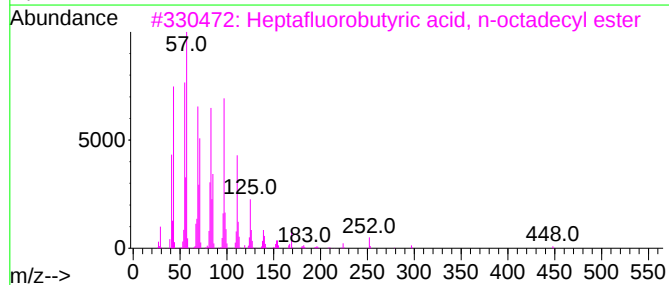
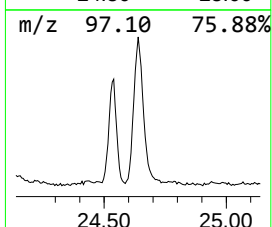
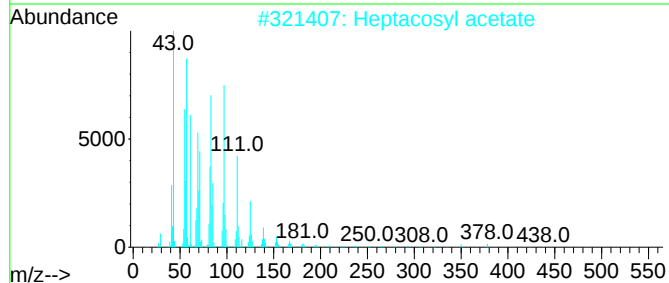
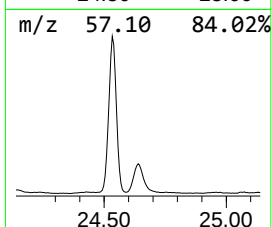
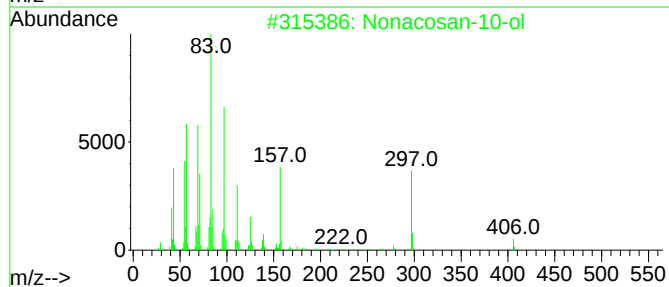
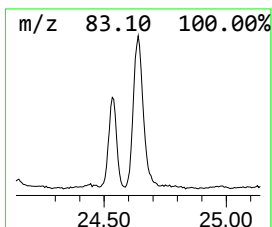
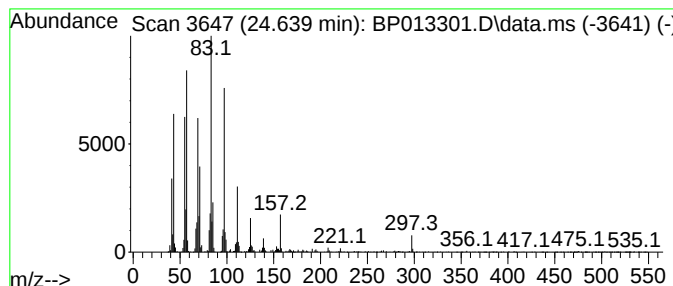
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Nonacosan-10-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.639	8.79 ng/ul	3369510	Perylene-d12	23.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosan-10-ol	424	C29H60O	000504-55-2	95
2			Heptacosyl acetate	438	C29H58O2	1000351-78-2	55
3			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	46
4			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	46
5			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013301.D
Acq On : 24 Dec 2022 15:49
Operator : CG/JU
Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

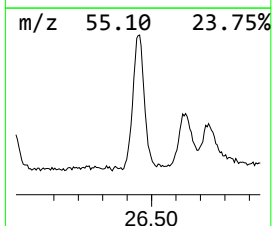
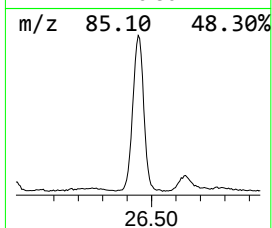
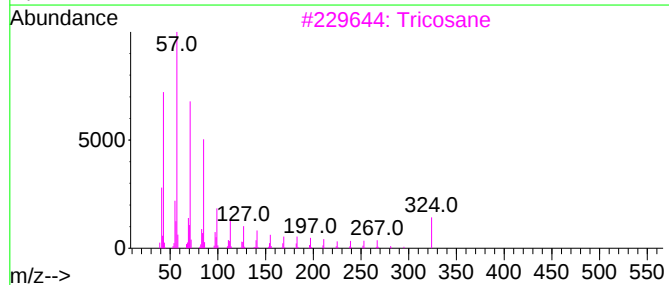
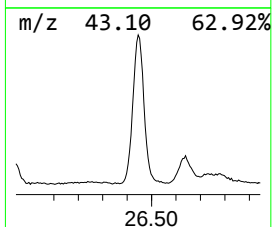
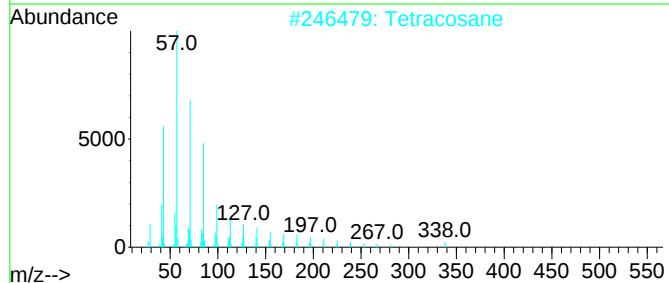
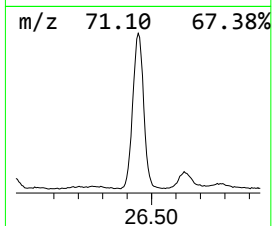
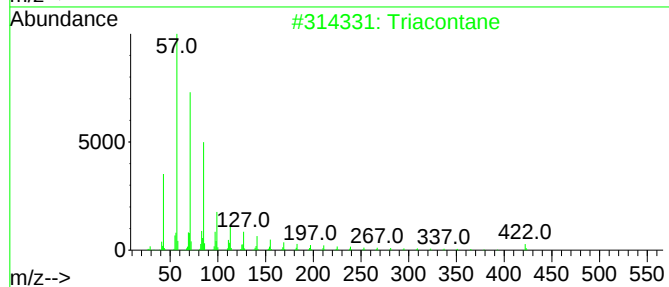
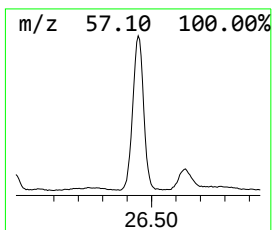
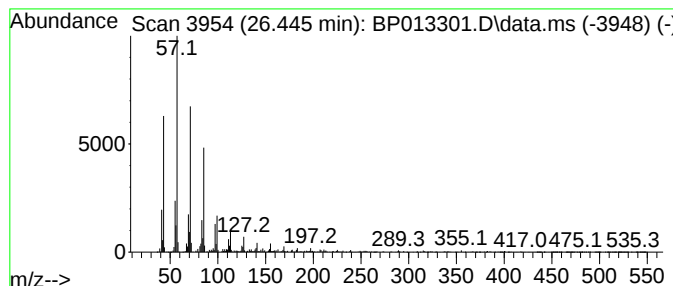
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
26.445	13.80 ng/ul	5288930	Perylene-d12		23.916	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Triacontane		422	C30H62	000638-68-6	98
2	Tetracosane		338	C24H50	000646-31-1	95
3	Tricosane		324	C23H48	000638-67-5	95
4	2-Methylheptacosane		394	C28H58	001561-00-8	91
5	Heptacosane		380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013301.D
Acq On : 24 Dec 2022 15:49
Operator : CG/JU
Sample : N6016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYD2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
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unknown-01	18.410	3.3	ng/ul	946855	4	17.345	5772760	20.0
3,5-di-tert-But...	19.828	3.5	ng/ul	1255850	5	21.433	7271930	20.0
Cinnamyl cinnamate	20.974	2.1	ng/ul	766028	5	21.433	7271930	20.0
(DEL) Alkane: C...	21.128	6.4	ng/ul	2338040	5	21.433	7271930	20.0
(DEL) Alkane: S...	23.127	5.8	ng/ul	2223760	6	23.916	7663080	20.0
(DEL) Alkane: S...	24.533	18.9	ng/ul	7256810	6	23.916	7663080	20.0
Nonacosan-10-ol	24.639	8.8	ng/ul	3369510	6	23.916	7663080	20.0
(DEL) Alkane: S...	26.445	13.8	ng/ul	5288930	6	23.916	7663080	20.0