

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121224\
 Data File : BP023406.D
 Acq On : 12 Dec 2024 21:53
 Operator : RC/JU
 Sample : P5232-12
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 E28S6

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-BP112624.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP023406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	16	19	29	rVB2	15674	25309	1.09%	0.089%
2	3.517	87	90	117	rVB	141731	275483	11.90%	0.968%
3	3.822	138	142	149	rVB3	7142	12905	0.56%	0.045%
4	4.311	223	225	230	rVB6	1937	2579	0.11%	0.009%
5	5.593	438	443	447	rVV6	2835	4539	0.20%	0.016%
6	5.693	457	460	463	rVB5	1765	2334	0.10%	0.008%
7	6.046	517	520	523	rBV4	1700	2538	0.11%	0.009%
8	6.752	633	640	658	rBV	196106	447869	19.35%	1.574%
9	6.887	658	663	676	rVB	177710	290853	12.57%	1.022%
10	7.087	691	697	711	rBV	227857	394997	17.07%	1.388%
11	7.534	763	773	788	rBV	381730	645303	27.88%	2.268%
12	8.257	890	896	914	rBV	159314	384062	16.59%	1.350%
13	8.681	962	968	988	rBV	228072	421191	18.20%	1.480%
14	9.057	1028	1032	1036	rBV7	4685	7334	0.32%	0.026%
15	9.246	1060	1064	1078	rBV3	17182	38911	1.68%	0.137%
16	9.393	1081	1089	1108	rBV	189561	390029	16.85%	1.371%
17	9.863	1166	1169	1173	rVB6	2236	2579	0.11%	0.009%
18	9.940	1175	1182	1208	rBV	245643	623075	26.92%	2.189%
19	10.281	1231	1240	1246	rBV	508705	871432	37.65%	3.062%
20	10.334	1246	1249	1260	rVB	35704	61852	2.67%	0.217%
21	10.440	1260	1267	1287	rBV	152511	391387	16.91%	1.375%
22	10.857	1334	1338	1343	rBV6	3872	6563	0.28%	0.023%
23	11.128	1381	1384	1389	rBV6	1648	3279	0.14%	0.012%
24	11.687	1471	1479	1485	rBV9	5173	7840	0.34%	0.028%
25	11.881	1508	1512	1519	rVB3	3224	6829	0.30%	0.024%
26	11.957	1521	1525	1533	rBV3	5294	11290	0.49%	0.040%
27	12.175	1556	1562	1569	rBV6	10120	26157	1.13%	0.092%
28	12.316	1582	1586	1588	rBV5	2717	3158	0.14%	0.011%
29	12.510	1616	1619	1624	rVV6	3049	4214	0.18%	0.015%
30	12.651	1640	1643	1648	rVB6	2729	5037	0.22%	0.018%
31	12.745	1655	1659	1662	rBV5	1827	3553	0.15%	0.012%
32	12.951	1687	1694	1701	rBV7	6882	14993	0.65%	0.053%
33	13.145	1717	1727	1750	rBV	255065	492032	21.26%	1.729%
34	13.463	1774	1781	1787	rBV	5208	11841	0.51%	0.042%
35	13.551	1788	1796	1804	rBV	713895	1010339	43.65%	3.550%
36	13.645	1810	1812	1819	rVB9	3763	5511	0.24%	0.019%

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Integrator: RTE

Smoothing : OFF

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Sampling : 1

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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-BP112624.MA.M
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37	13.839	1838	1845	1866	rVB	689717	1018637	44.01%	3.579%
38	14.045	1873	1880	1884	rVB5	8696	14157	0.61%	0.050%
39	14.151	1887	1898	1907	rBV	850324	1351963	58.41%	4.751%
40	14.463	1944	1951	1977	rBV3	108947	456005	19.70%	1.602%
41	14.781	2003	2005	2012	rVB8	4553	6237	0.27%	0.022%
42	14.851	2013	2017	2018	rBV4	3219	4281	0.18%	0.015%
43	14.951	2031	2034	2038	rVV6	3042	5091	0.22%	0.018%
44	15.010	2041	2044	2049	rVB7	6973	10576	0.46%	0.037%
45	15.163	2064	2070	2084	rBV	775452	1278384	55.23%	4.492%
46	15.263	2084	2087	2092	rVB7	3222	4095	0.18%	0.014%
47	15.322	2092	2097	2105	rBV2	150534	291373	12.59%	1.024%
48	15.434	2114	2116	2121	rVB6	5697	5734	0.25%	0.020%
49	15.539	2128	2134	2144	rBV	366492	491077	21.22%	1.726%
50	15.922	2191	2199	2204	rBV5	13912	32204	1.39%	0.113%
51	15.998	2210	2212	2216	rVB5	5775	6568	0.28%	0.023%
52	16.051	2217	2221	2227	rVV8	16431	28085	1.21%	0.099%
53	16.122	2229	2233	2239	rVB9	7786	13154	0.57%	0.046%
54	16.351	2268	2272	2277	rBV4	16849	25572	1.10%	0.090%
55	16.481	2290	2294	2301	rBV8	5159	11175	0.48%	0.039%
56	16.551	2305	2306	2310	rVB4	2500	2577	0.11%	0.009%
57	16.610	2310	2316	2323	rBV4	13846	37611	1.62%	0.132%
58	16.704	2329	2332	2339	rBV7	6901	11748	0.51%	0.041%
59	16.869	2355	2360	2367	rBV	55539	79301	3.43%	0.279%
60	16.957	2367	2375	2380	rVV2	1121940	1807433	78.09%	6.351%
61	16.998	2380	2382	2386	rVV	66151	87100	3.76%	0.306%
62	17.051	2386	2391	2405	rVB	928695	1375812	59.44%	4.835%
63	17.157	2405	2409	2413	rBV7	11515	17245	0.75%	0.061%
64	17.245	2422	2424	2426	rBV3	3320	3664	0.16%	0.013%
65	17.322	2435	2437	2439	rBV3	5023	5415	0.23%	0.019%
66	17.375	2443	2446	2449	rVV5	7612	11386	0.49%	0.040%
67	17.592	2480	2483	2485	rBV4	7068	9180	0.40%	0.032%
68	17.622	2485	2488	2490	rVV4	8137	11482	0.50%	0.040%
69	17.645	2490	2492	2497	rVB5	13559	17089	0.74%	0.060%
70	17.763	2505	2512	2517	rBV3	66068	134169	5.80%	0.471%
71	17.828	2517	2523	2529	rVV	526467	1002254	43.30%	3.522%
72	17.892	2529	2534	2552	rVB	1177614	1779071	76.87%	6.252%
73	18.051	2559	2561	2567	rVB6	12879	19154	0.83%	0.067%
74	18.204	2584	2587	2592	rVB6	34332	49740	2.15%	0.175%
75	18.333	2605	2609	2614	rVB5	18649	28287	1.22%	0.099%
76	18.386	2616	2618	2620	rBV2	8771	7392	0.32%	0.026%

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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

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Peak separation: 5

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Title : SVOA CALIBRATION

77	18.445	2625	2628	2636	rVB3	32750	55695	2.41%	0.196%
78	18.751	2677	2680	2685	rBV5	11309	18634	0.81%	0.065%
79	18.975	2715	2718	2723	rVB6	16715	23465	1.01%	0.082%
80	19.098	2730	2739	2753	rBV	364310	907642	39.21%	3.189%
81	19.227	2757	2761	2770	rVV	250101	347078	15.00%	1.220%
82	19.439	2791	2797	2813	rBV2	972746	1779985	76.90%	6.255%
83	21.057	3067	3072	3082	rBV6	182644	459804	19.87%	1.616%
84	21.374	3120	3126	3143	rBV2	1208548	2314532	100.00%	8.133%
85	23.063	3408	3413	3423	rVB	176467	341128	14.74%	1.199%
86	24.327	3621	3628	3637	rVB	501581	1182515	51.09%	4.155%
87	24.545	3656	3665	3686	rVB	751059	2230779	96.38%	7.839%
88	31.709	4876	4883	4885	rBV6	146950	335982	14.52%	1.181%

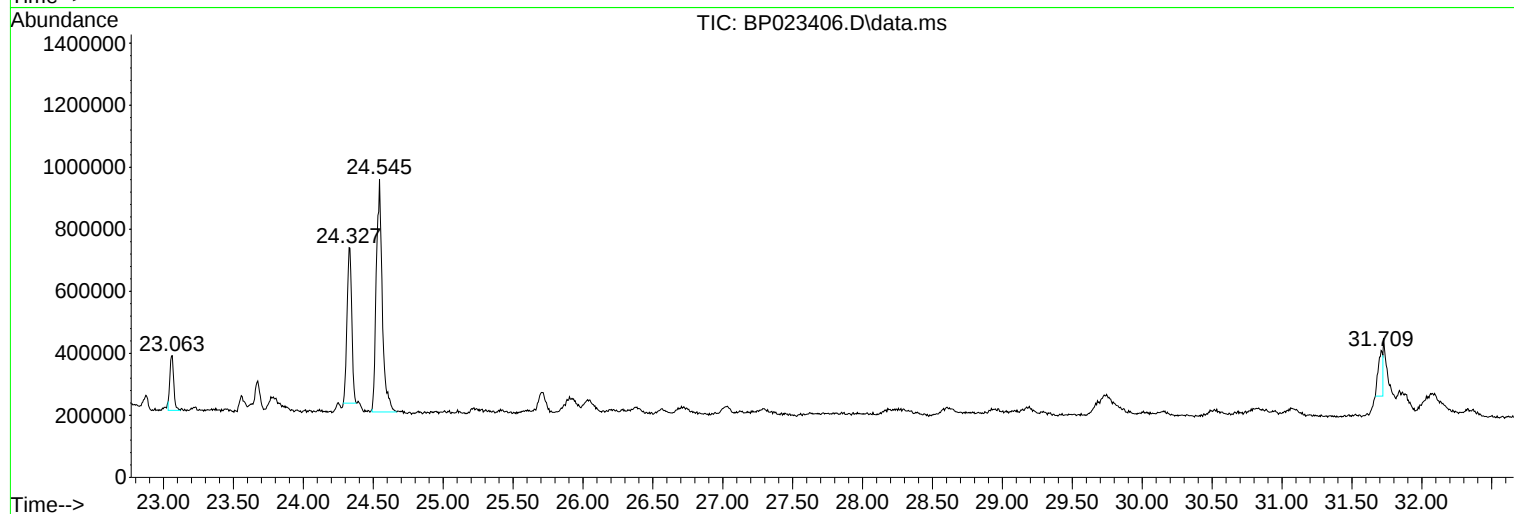
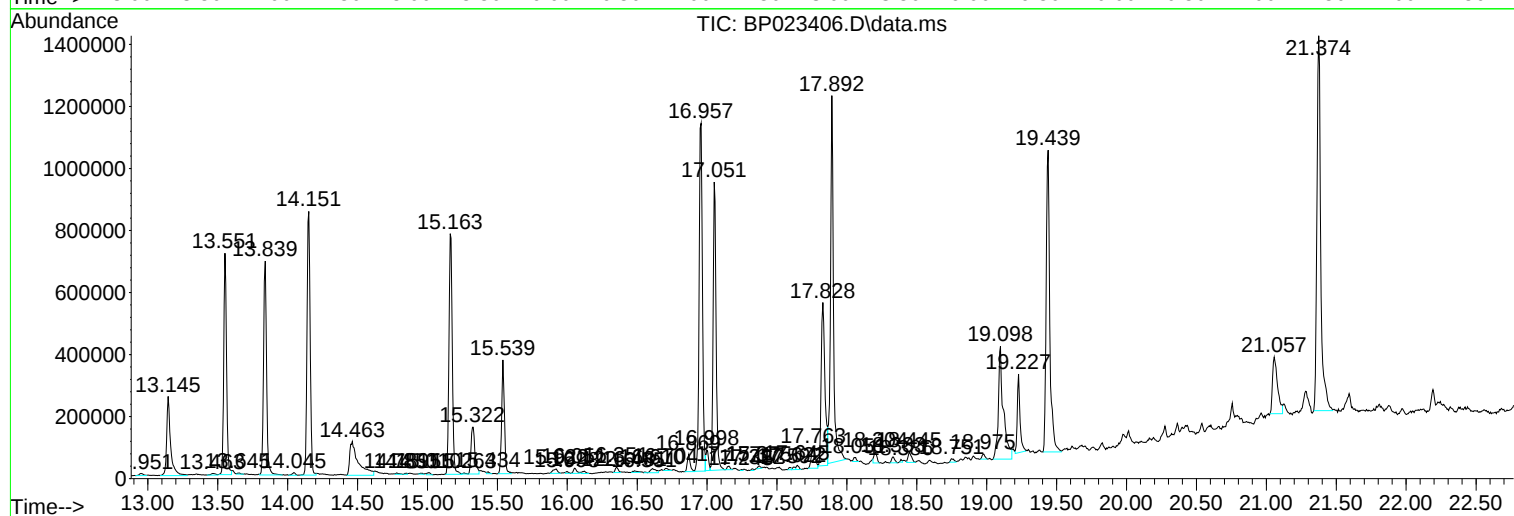
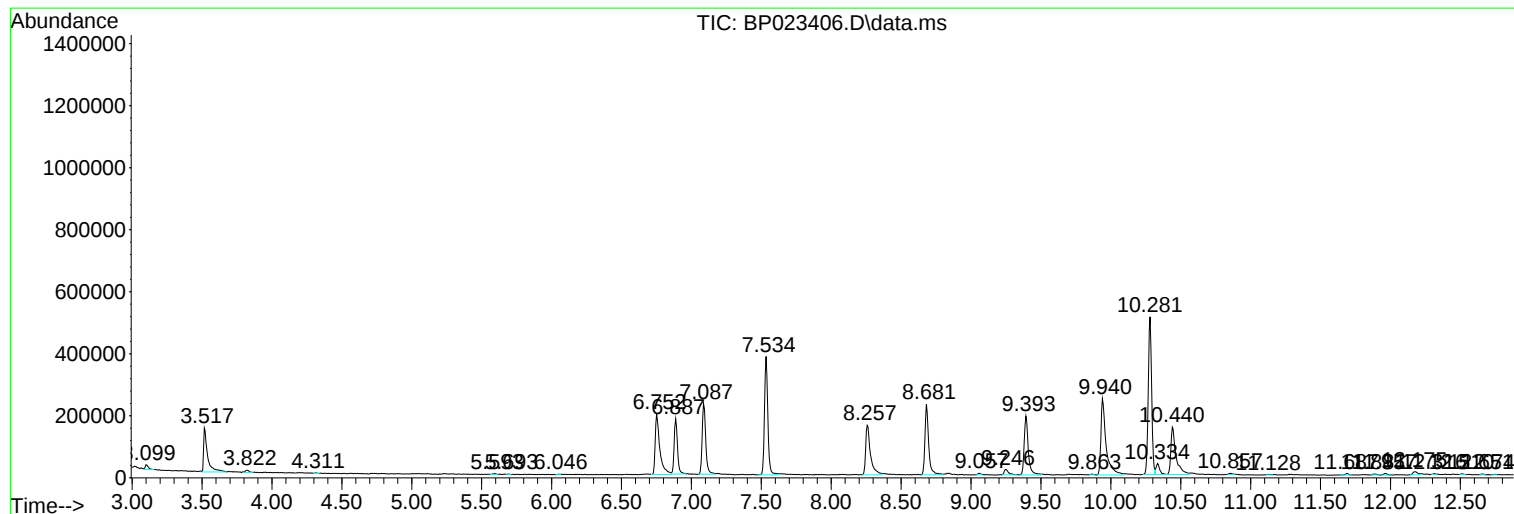
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.MA.M
Quant Title : SVOA CALIBRATION

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



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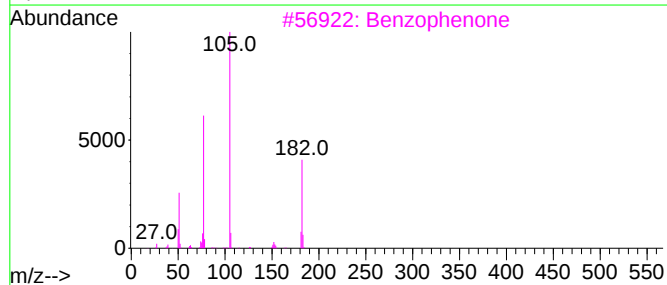
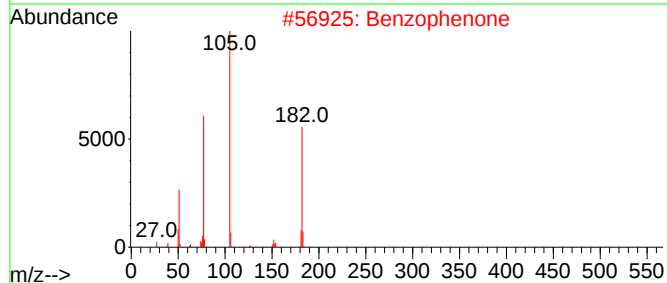
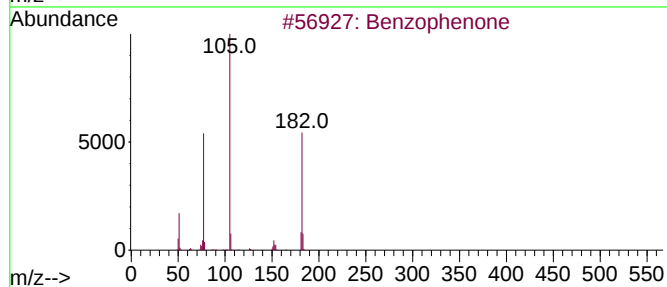
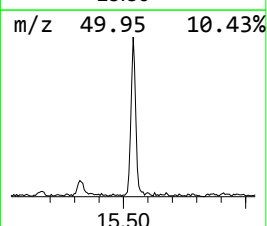
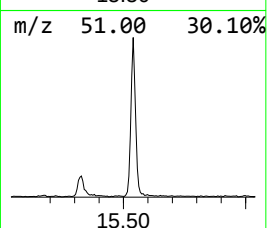
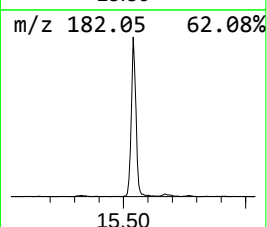
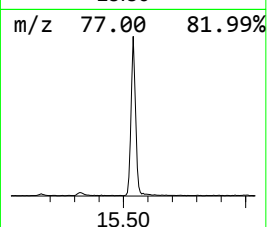
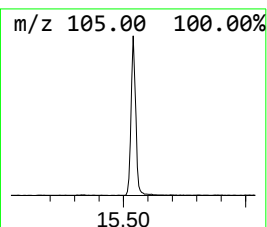
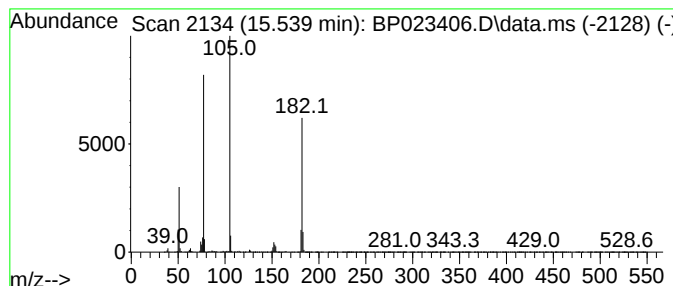
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.539	7.26 ng/ul	491077	Acenaphthene-d10	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	94
4			Benzophenone	182	C13H10O	000119-61-9	87
5			Benzophenone	182	C13H10O	000119-61-9	83



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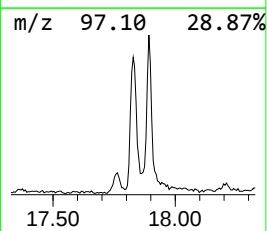
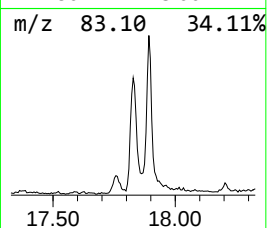
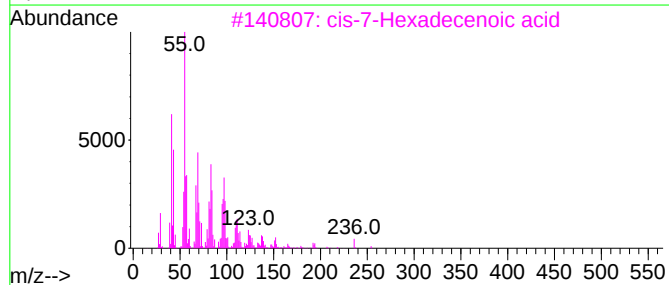
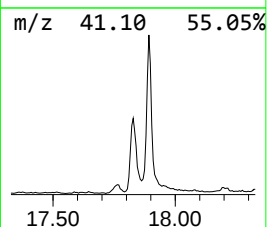
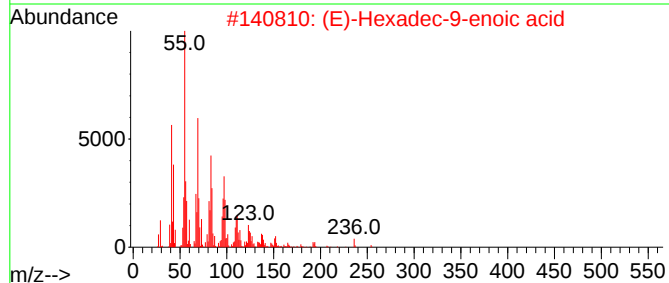
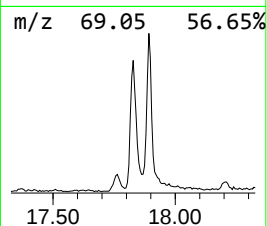
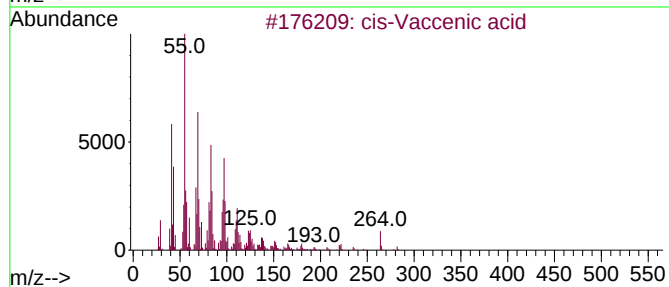
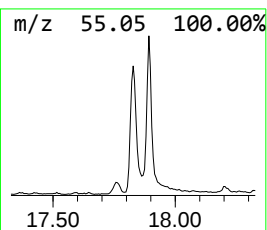
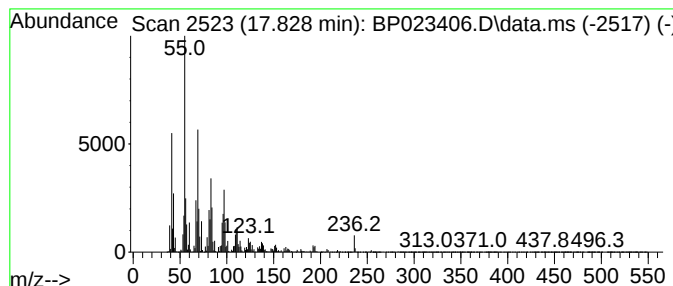
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.828	11.09 ng/ul	1002250	Phenanthrene-d10	16.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
3			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	98
4			Palmitoleic acid	254	C16H30O2	000373-49-9	96
5			Palmitoleic acid	254	C16H30O2	000373-49-9	95



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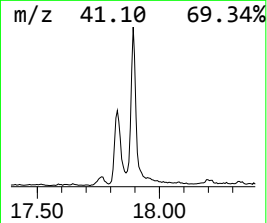
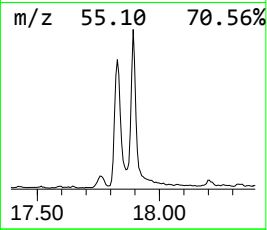
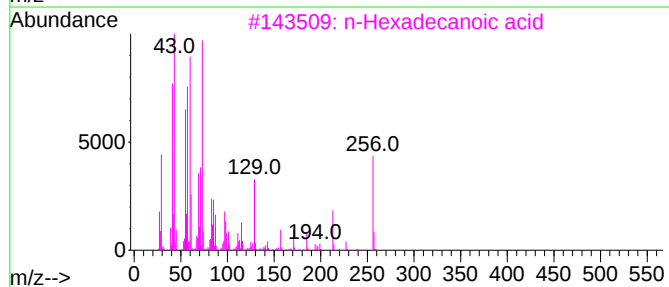
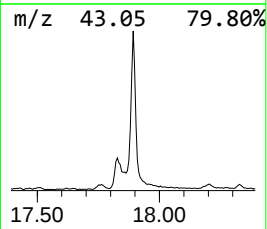
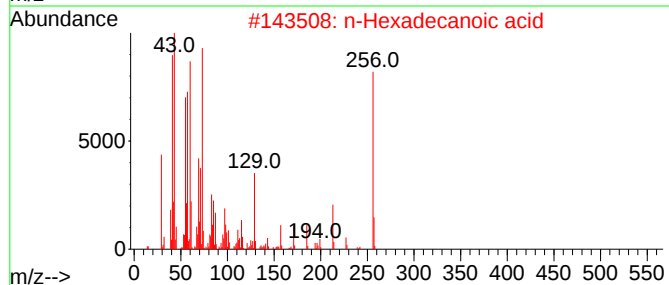
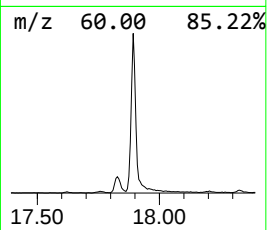
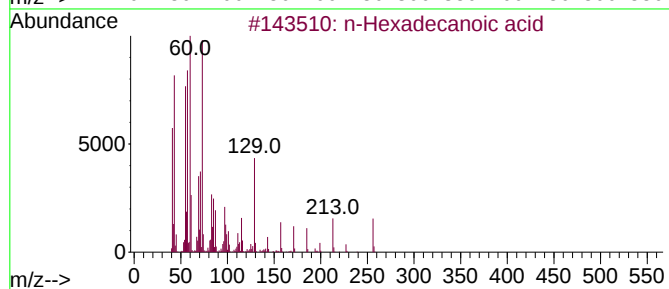
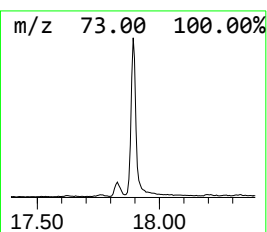
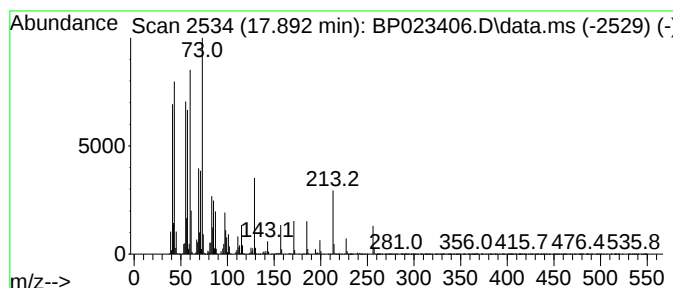
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.892	19.69 ng/ul	1779070	Phenanthrene-d10	16.951	
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	Tridecanoic acid	214	C13H26O2	000638-53-9	91



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E28S6

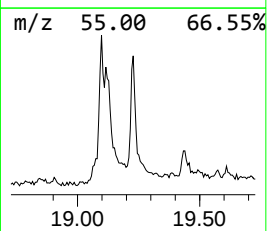
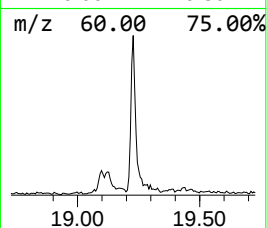
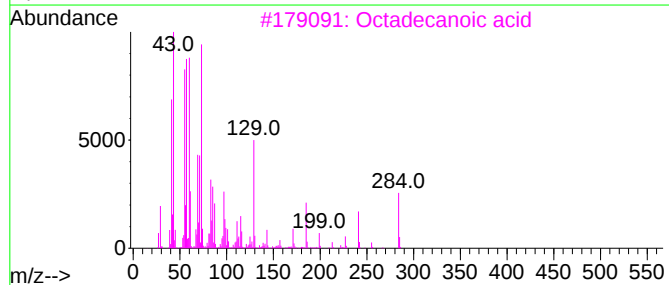
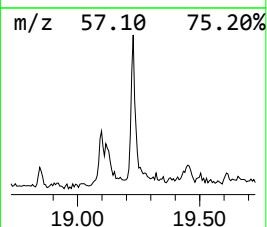
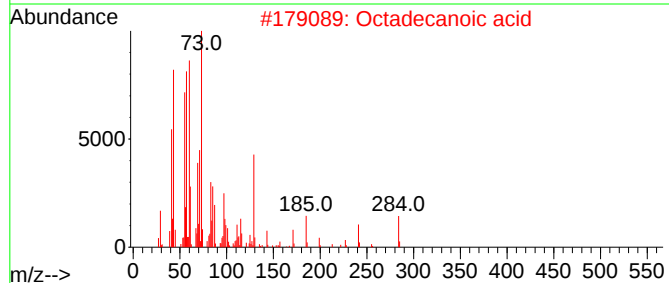
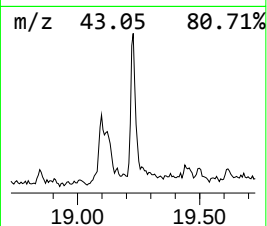
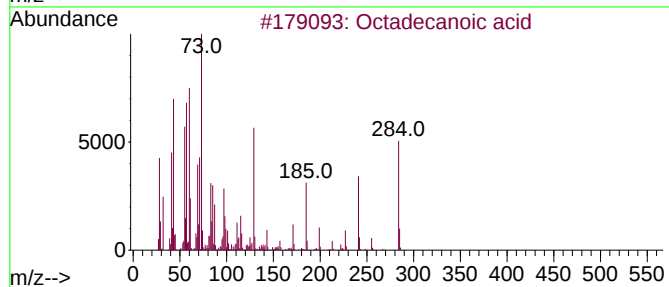
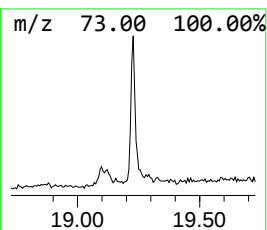
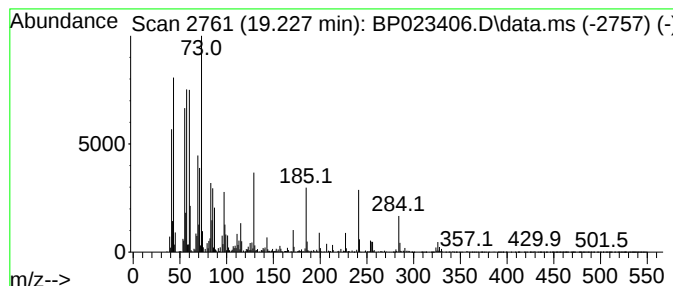
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	3.00 ng/ul	347078	Chrysene-d12	21.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	97
4			Octadecanoic acid	284	C18H36O2	000057-11-4	95
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121224\
Data File : BP023406.D
Acq On : 12 Dec 2024 21:53
Operator : RC/JU
Sample : P5232-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E28S6

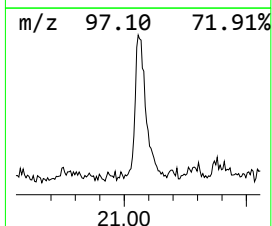
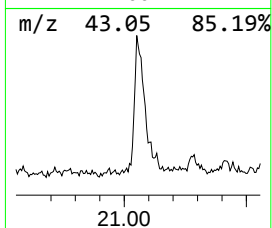
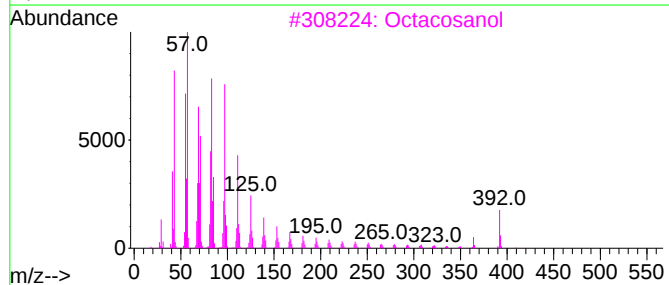
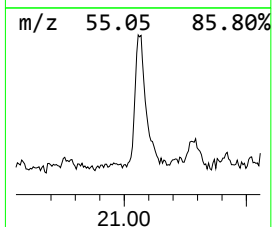
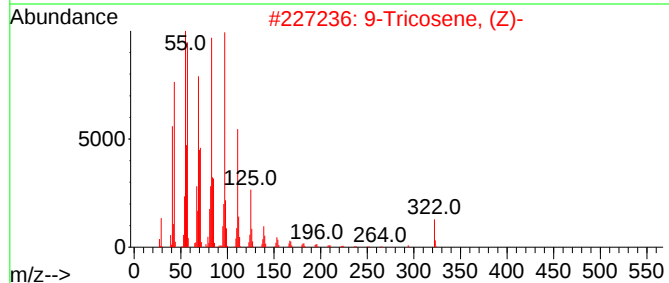
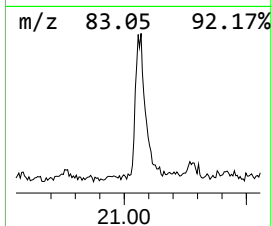
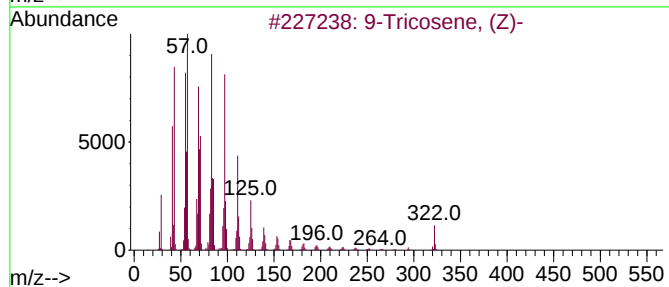
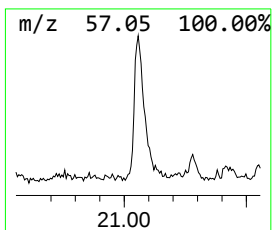
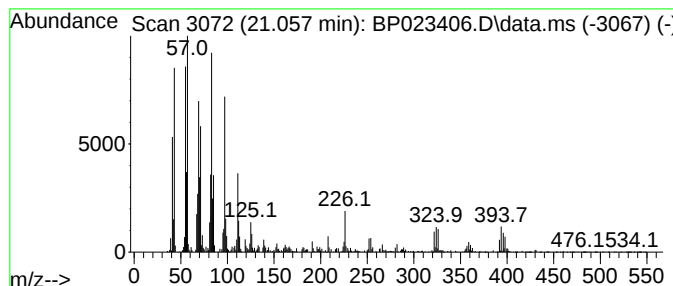
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Quant Title : SVOA CALIBRATION

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.
21.057	3.97 ng/ul	459804	Chrysene-d12	21.374

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91	
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	90	
3	Octacosanol	410	C28H58O	000557-61-9	90	
4	2-Methyl-2-docosene	322	C23H46	1000131-16-9	64	
5	5-Methyl-Z-5-docosene	322	C23H46	1000131-17-1	56	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121224\
Data File : BP023406.D
Acq On : 12 Dec 2024 21:53
Operator : RC/JU
Sample : P5232-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E28S6

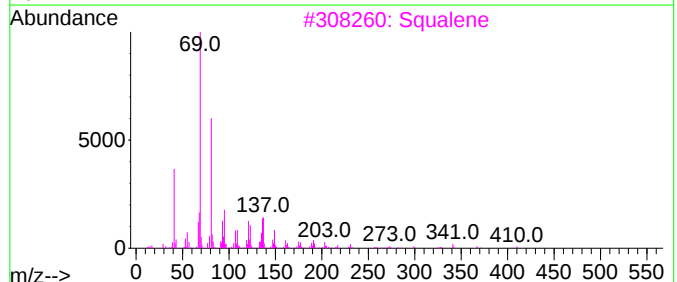
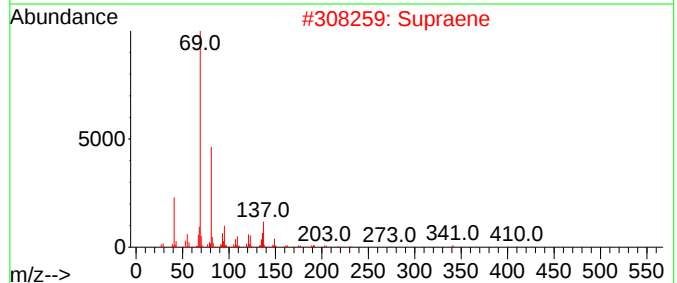
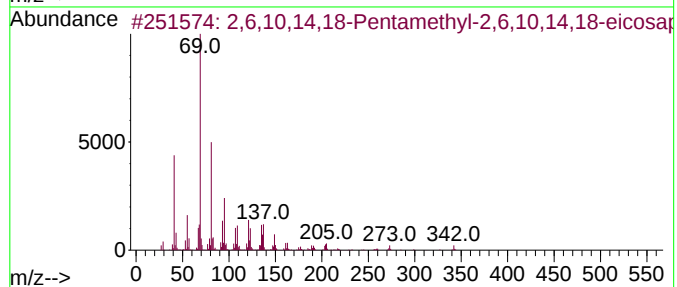
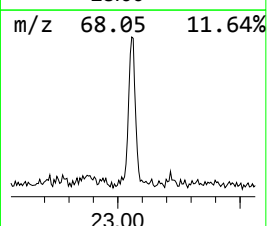
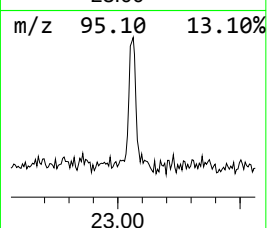
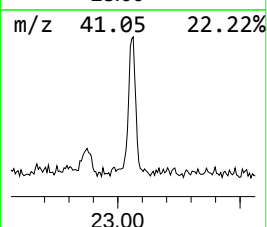
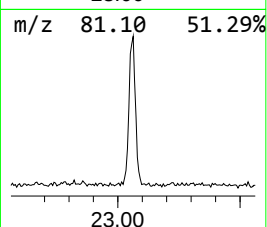
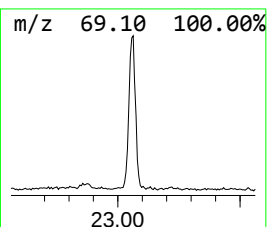
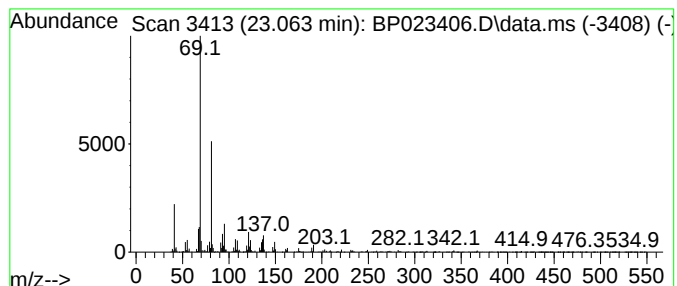
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.063	3.06 ng/ul	341128	Perylene-d12	24.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	93		
2	Supraene	410	C30H50	007683-64-9	83		
3	Squalene	410	C30H50	000111-02-4	80		
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68		
5	Umbelliprenin	366	C24H30O3	023838-17-7	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121224\
Data File : BP023406.D
Acq On : 12 Dec 2024 21:53
Operator : RC/JU
Sample : P5232-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E28S6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112624.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
Benzophenone	15.539	7.3	ng/ul	491077	3	14.151	1351960	20.0
cis-Vaccenic acid	17.828	11.1	ng/ul	1002250	4	16.951	1807430	20.0
n-Hexadecanoic ...	17.892	19.7	ng/ul	1779070	4	16.951	1807430	20.0
Octadecanoic acid	19.227	3.0	ng/ul	347078	5	21.374	2314530	20.0
(DEL) Alkane: S...	21.057	4.0	ng/ul	459804	5	21.374	2314530	20.0
2,6,10,14,18-Pe...	23.063	3.1	ng/ul	341128	6	24.545	2230780	20.0