

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
 Data File : BP015594.D
 Acq On : 16 Jun 2023 23:07
 Operator : MA/JU
 Sample : 03080-06
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFH5

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-BP060723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.405	34	37	43	rVB2	11654	15275	0.53%	0.039%
2	3.858	111	114	125	rBV	93478	174117	6.09%	0.442%
3	3.958	128	131	137	rVB5	13826	21502	0.75%	0.055%
4	4.081	147	152	158	rVB	15440	29047	1.02%	0.074%
5	4.175	165	168	174	rVB3	8052	11516	0.40%	0.029%
6	5.134	327	331	335	rVB4	4117	6929	0.24%	0.018%
7	6.052	481	487	494	rBV4	3801	9650	0.34%	0.025%
8	6.305	525	530	536	rVV4	8631	17498	0.61%	0.044%
9	7.099	662	665	669	rBV5	3153	5708	0.20%	0.014%
10	7.240	679	689	707	rVB2	230321	639456	22.38%	1.624%
11	7.405	710	717	730	rVB	179279	300706	10.52%	0.764%
12	7.610	745	752	761	rBV	235250	393456	13.77%	0.999%
13	7.681	761	764	768	rVB4	6587	9242	0.32%	0.023%
14	8.081	822	832	844	rBV	491752	805972	28.21%	2.047%
15	8.346	874	877	882	rBV7	3220	6778	0.24%	0.017%
16	8.804	948	955	966	rBV	195223	379481	13.28%	0.964%
17	8.928	971	976	982	rVB	14147	27107	0.95%	0.069%
18	9.187	1015	1020	1025	rVB9	2843	5752	0.20%	0.015%
19	9.263	1025	1033	1047	rBV	222084	416760	14.59%	1.059%
20	9.634	1092	1096	1102	rVB8	4283	9319	0.33%	0.024%
21	9.987	1149	1156	1168	rBV	188703	354490	12.41%	0.900%
22	10.257	1192	1202	1206	rBV	4297	10276	0.36%	0.026%
23	10.293	1206	1208	1217	rVB9	2427	5361	0.19%	0.014%
24	10.534	1243	1249	1277	rBV	230542	535657	18.75%	1.361%
25	10.910	1305	1313	1319	rBV	710791	1210212	42.36%	3.074%
26	11.057	1331	1338	1357	rBV	127870	339805	11.89%	0.863%
27	11.728	1446	1452	1455	rBV8	5331	7878	0.28%	0.020%
28	11.916	1478	1484	1488	rBV6	5323	10286	0.36%	0.026%
29	12.304	1546	1550	1555	rBV8	4503	8174	0.29%	0.021%
30	12.498	1576	1583	1590	rVB8	5562	11321	0.40%	0.029%
31	12.569	1590	1595	1600	rBV4	7497	12059	0.42%	0.031%
32	12.651	1603	1609	1620	rBV4	11531	40470	1.42%	0.103%
33	12.787	1627	1632	1637	rVB4	7118	11165	0.39%	0.028%
34	13.081	1677	1682	1685	rVV7	3707	7255	0.25%	0.018%
35	13.245	1706	1710	1715	rVB7	6201	8174	0.29%	0.021%
36	13.322	1718	1723	1728	rVB8	3852	6574	0.23%	0.017%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
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37	13.457	1742	1746	1747	rVV4	6252	7288	0.26%	0.019%
38	13.487	1747	1751	1755	rVB6	7036	11411	0.40%	0.029%
39	13.534	1755	1759	1762	rBV6	7030	10193	0.36%	0.026%
40	13.610	1767	1772	1780	rVB3	26329	46155	1.62%	0.117%
41	13.910	1814	1823	1828	rBV10	6760	19451	0.68%	0.049%
42	14.045	1841	1846	1852	rBV6	11718	20650	0.72%	0.052%
43	14.134	1852	1861	1867	rVV	589467	850893	29.78%	2.161%
44	14.187	1867	1870	1877	rVB8	9695	15030	0.53%	0.038%
45	14.422	1902	1910	1924	rBV2	657619	1009193	35.32%	2.563%
46	14.604	1938	1941	1946	rVB4	12147	17464	0.61%	0.044%
47	14.686	1949	1955	1956	rBV6	6532	10714	0.37%	0.027%
48	14.728	1956	1962	1968	rVV	1164652	1712563	59.94%	4.350%
49	14.781	1968	1971	1979	rVB6	31016	56877	1.99%	0.144%
50	14.963	1994	2002	2008	rBV2	69629	179357	6.28%	0.456%
51	15.128	2025	2030	2037	rBV7	14311	28092	0.98%	0.071%
52	15.198	2040	2042	2048	rVB7	6593	9481	0.33%	0.024%
53	15.504	2088	2094	2098	rBV9	10249	17118	0.60%	0.043%
54	15.551	2098	2102	2106	rVB4	10832	18543	0.65%	0.047%
55	15.722	2124	2131	2136	rBV	818010	1224581	42.86%	3.110%
56	15.851	2147	2153	2166	rBV	186001	325575	11.39%	0.827%
57	16.086	2187	2193	2201	rBV	86055	138403	4.84%	0.352%
58	16.169	2205	2207	2210	rBV4	6398	8782	0.31%	0.022%
59	16.416	2246	2249	2250	rBV2	17996	18547	0.65%	0.047%
60	16.863	2322	2325	2330	rVB5	19627	28043	0.98%	0.071%
61	17.139	2368	2372	2377	rBV6	12820	21513	0.75%	0.055%
62	17.216	2381	2385	2391	rVB4	21483	31749	1.11%	0.081%
63	17.298	2397	2399	2405	rVB3	9950	14036	0.49%	0.036%
64	17.357	2405	2409	2416	rBV2	37450	57814	2.02%	0.147%
65	17.422	2417	2420	2425	rVV3	28563	37655	1.32%	0.096%
66	17.480	2425	2430	2435	rVV	1480953	2124345	74.35%	5.396%
67	17.522	2435	2437	2442	rVV	202160	279956	9.80%	0.711%
68	17.580	2442	2447	2461	rVB	860569	1331518	46.60%	3.382%
69	17.751	2474	2476	2478	rBV3	7889	7233	0.25%	0.018%
70	17.886	2496	2499	2505	rVB2	25341	39662	1.39%	0.101%
71	17.945	2506	2509	2514	rVB	20943	26016	0.91%	0.066%
72	18.127	2537	2540	2545	rVB6	24665	29265	1.02%	0.074%
73	18.227	2554	2557	2561	rVB3	28270	35101	1.23%	0.089%
74	18.286	2563	2567	2571	rBV	95554	124513	4.36%	0.316%
75	18.339	2571	2576	2582	rBV	1029378	1368454	47.89%	3.476%
76	18.622	2620	2624	2631	rBV5	48351	102581	3.59%	0.261%

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77	18.822	2655	2658	2662	rBV4	34050	55981	1.96%	0.142%
78	18.869	2664	2666	2672	rVB3	49346	66952	2.34%	0.170%
79	19.222	2723	2726	2730	rVB2	69480	75178	2.63%	0.191%
80	19.427	2758	2761	2763	rBV	94420	115677	4.05%	0.294%
81	19.480	2763	2770	2776	rVB	633935	999392	34.98%	2.538%
82	19.563	2780	2784	2792	rVV	393714	528274	18.49%	1.342%
83	19.804	2820	2825	2828	rBV	1338136	1776498	62.18%	4.512%
84	19.833	2828	2830	2834	rVB	445559	472668	16.54%	1.201%
85	20.298	2906	2909	2917	rVB3	95778	146426	5.12%	0.372%
86	20.610	2959	2962	2966	rBV4	90095	115931	4.06%	0.294%
87	21.245	3065	3070	3075	rBV2	364637	593649	20.78%	1.508%
88	21.445	3101	3104	3108	rVB2	159973	196770	6.89%	0.500%
89	21.563	3118	3124	3128	rBV2	1859495	2857238	100.00%	7.257%
90	21.604	3128	3131	3135	rVB	265598	338364	11.84%	0.859%
91	22.163	3224	3226	3230	rVB	246758	260339	9.11%	0.661%
92	22.957	3357	3361	3367	rBV	405265	598872	20.96%	1.521%
93	23.280	3411	3416	3421	rBV	926682	1507093	52.75%	3.828%
94	23.357	3425	3429	3443	rVB2	820434	2097256	73.40%	5.327%
95	23.945	3523	3529	3535	rBV3	862470	1702394	59.58%	4.324%
96	24.110	3551	3557	3564	rVB	1074413	2142106	74.97%	5.441%
97	24.615	3639	3643	3652	rVB6	328751	670503	23.47%	1.703%
98	24.733	3656	3663	3676	rVB	1090299	2458412	86.04%	6.244%
99	26.186	3906	3910	3923	rVB2	420031	1033423	36.17%	2.625%
100	26.715	3993	4000	4008	rBV	438323	1280673	44.82%	3.253%

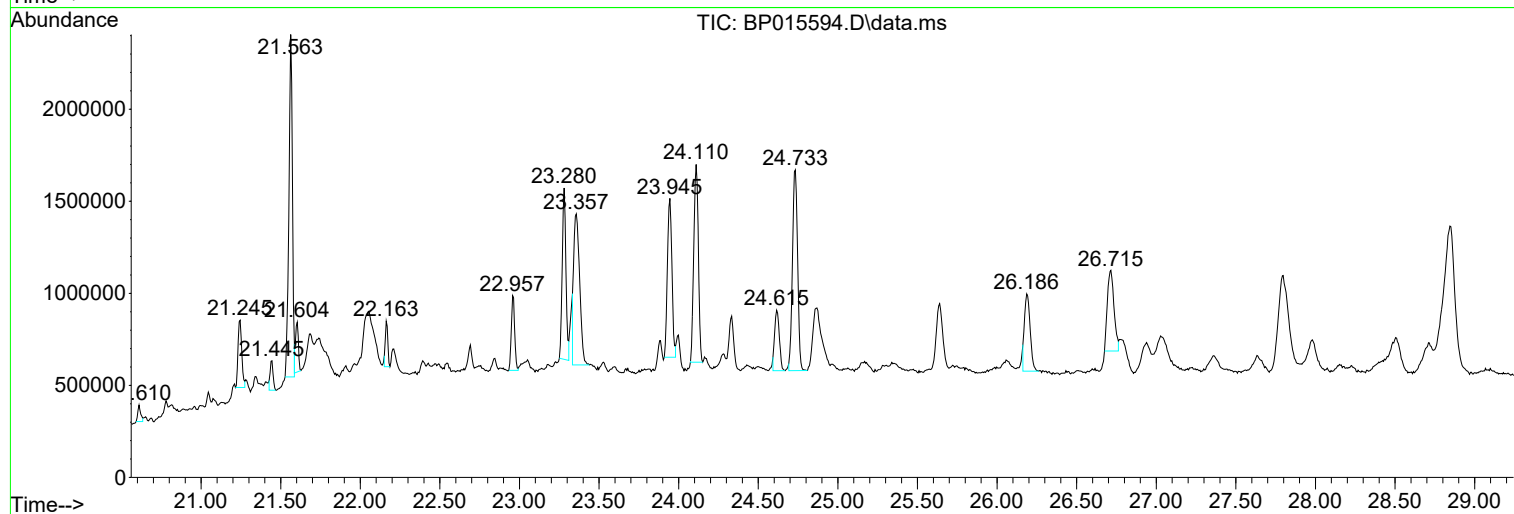
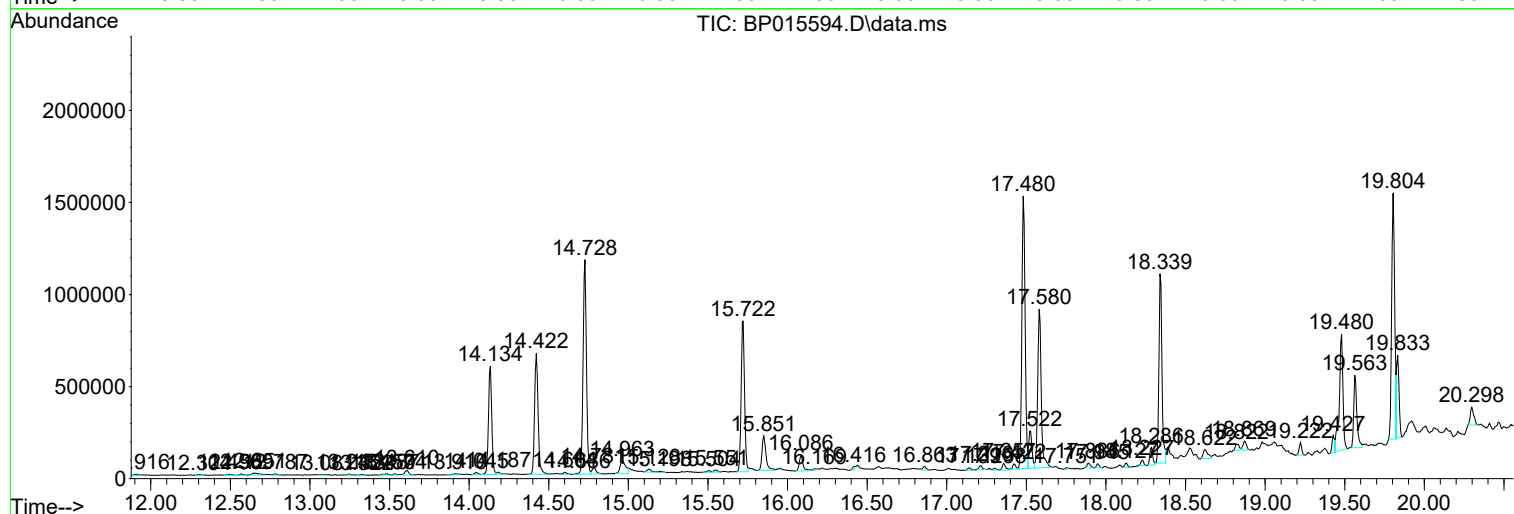
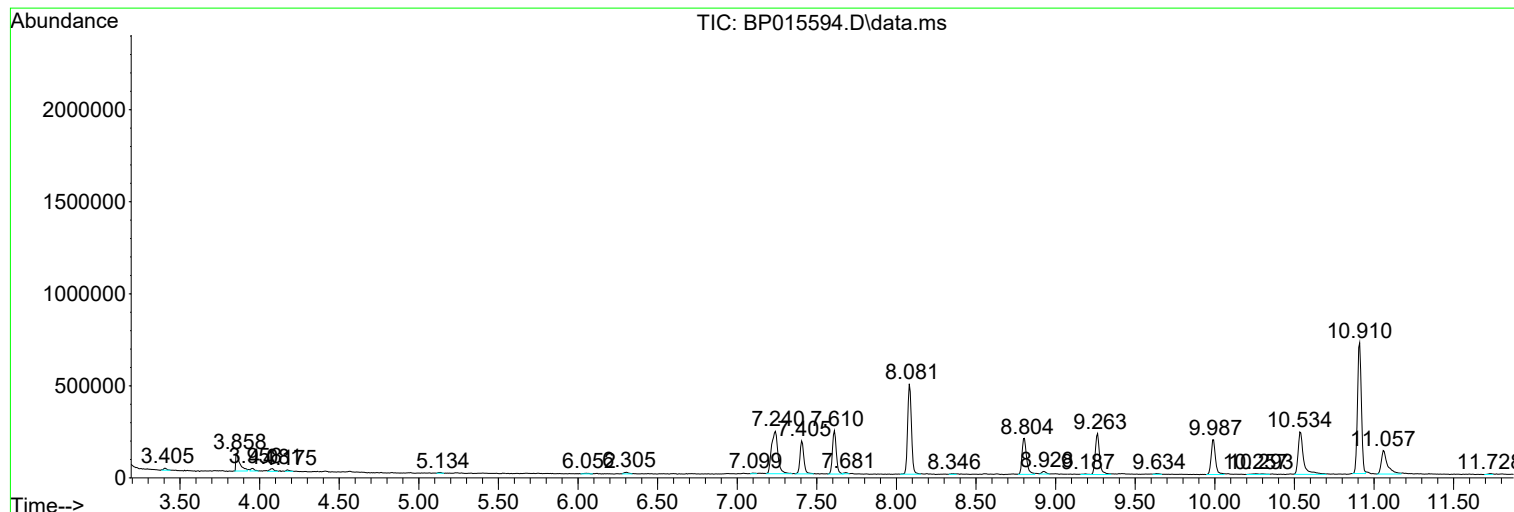
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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



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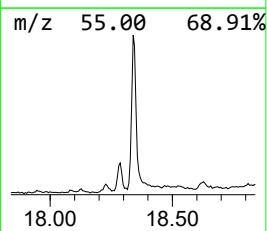
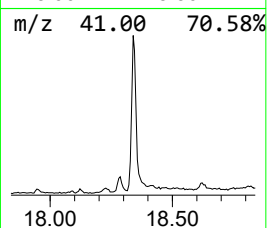
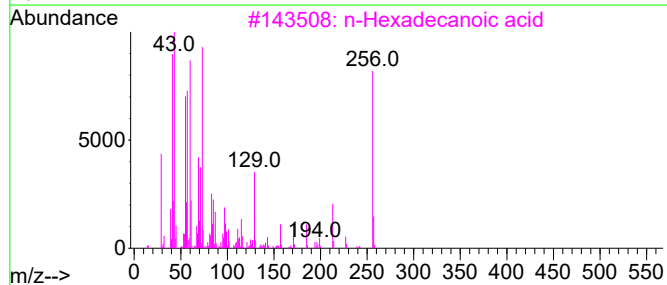
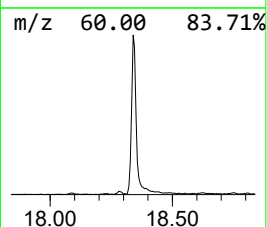
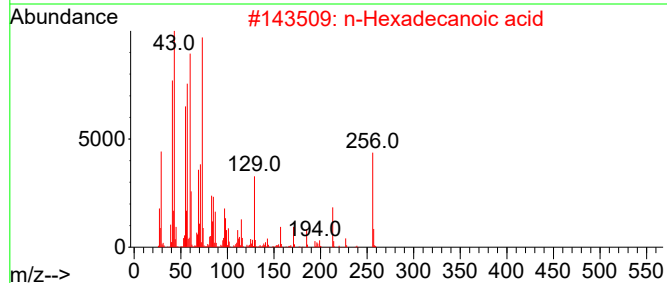
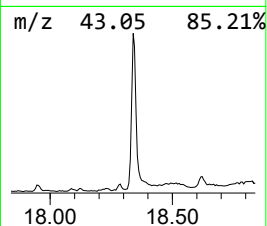
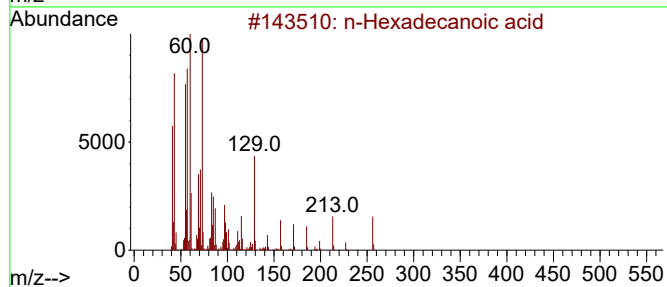
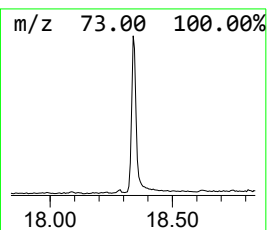
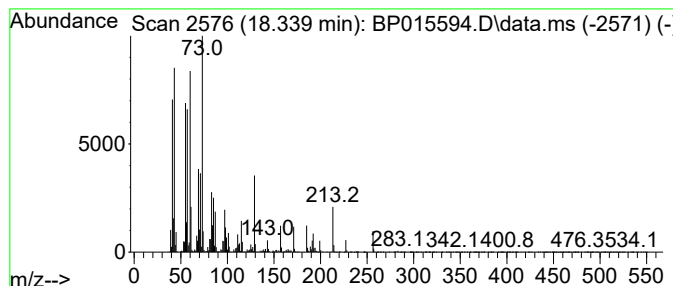
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.339	12.88 ng/ul	1368450	Phenanthrene-d10	17.480

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	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95



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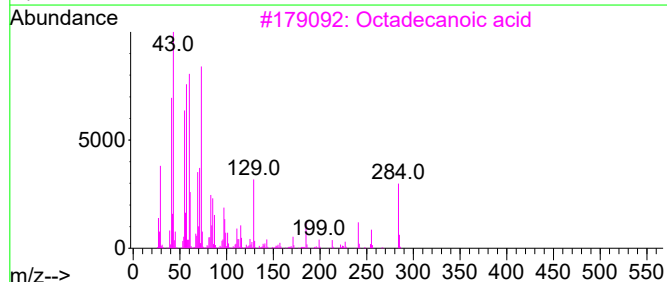
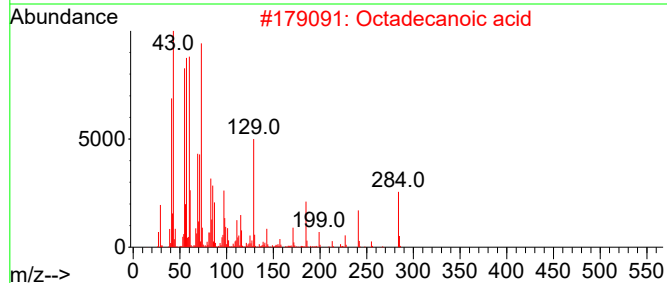
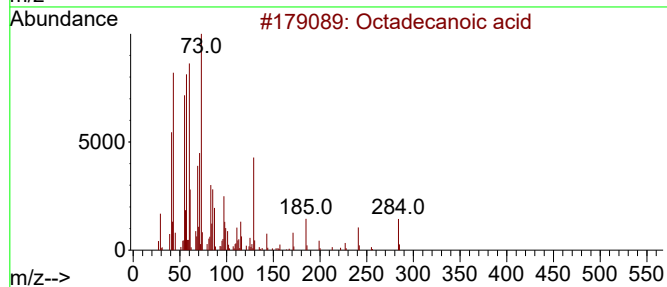
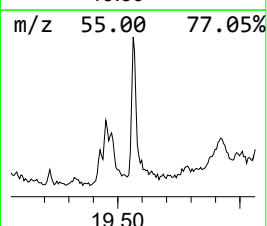
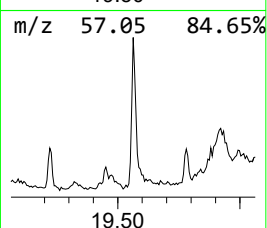
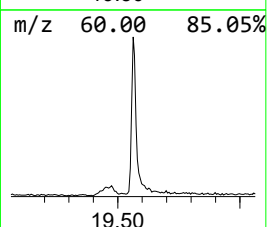
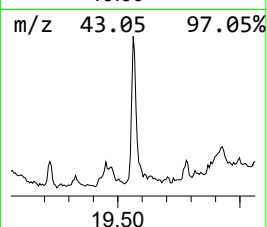
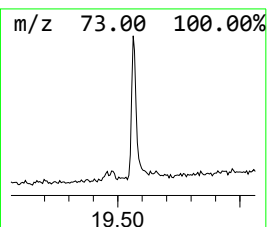
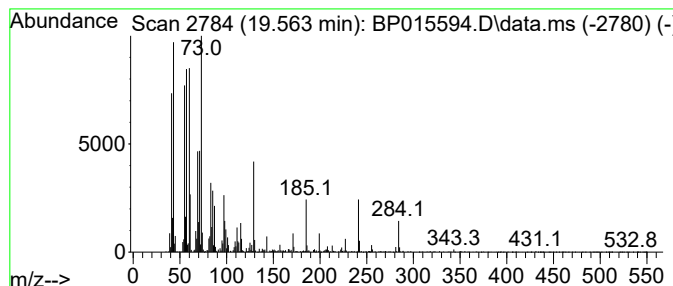
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.563	3.70 ng/ul	528274	Chrysene-d12	21.563

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	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



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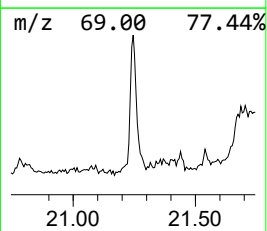
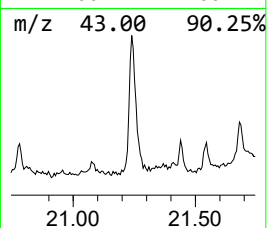
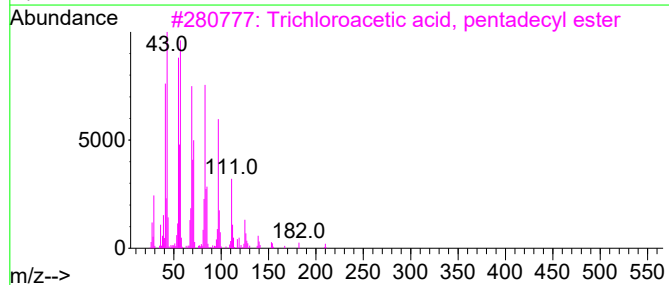
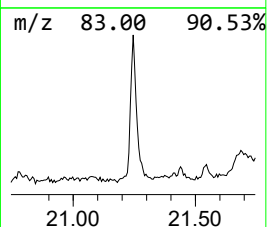
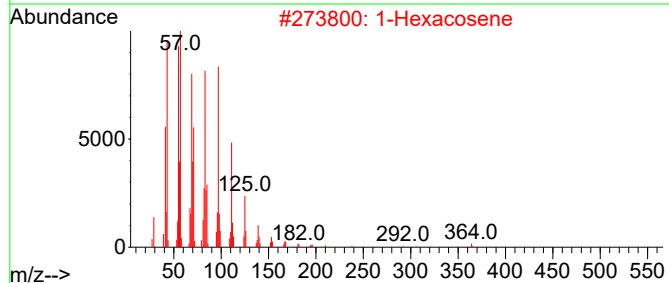
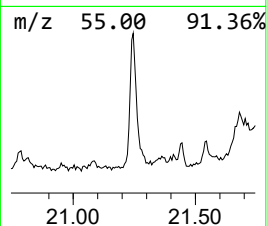
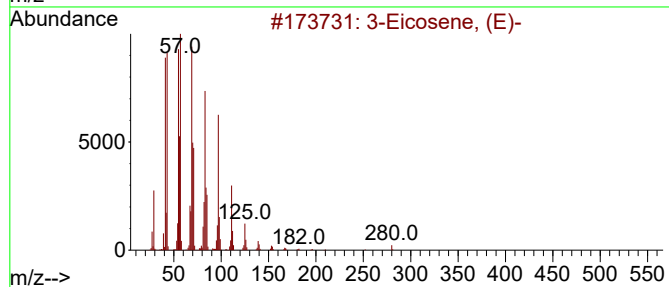
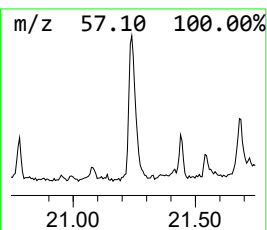
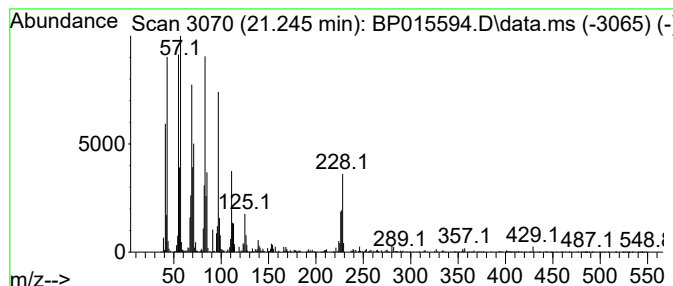
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	4.16 ng/ul	593649	Chrysene-d12	21.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-			280	C20H40	074685-33-9	96
2	1-Hexacosene			364	C26H52	018835-33-1	93
3	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	93
4	9-Eicosene, (E)-			280	C20H40	074685-29-3	91
5	1-Octadecene			252	C18H36	000112-88-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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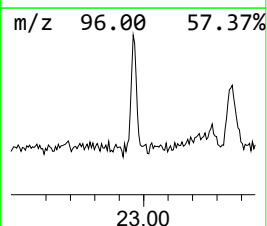
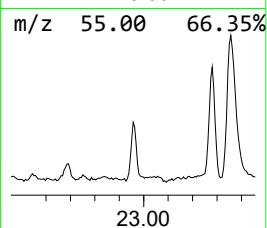
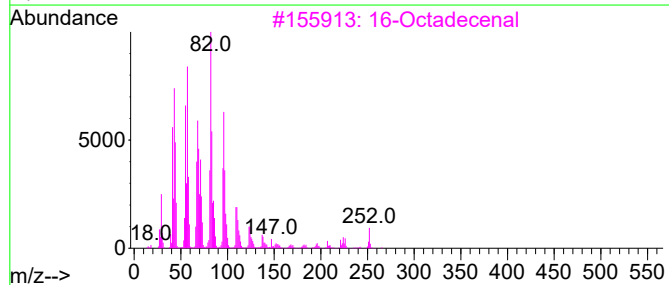
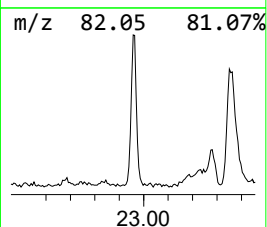
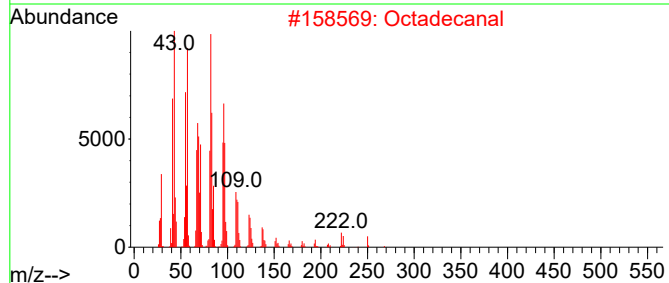
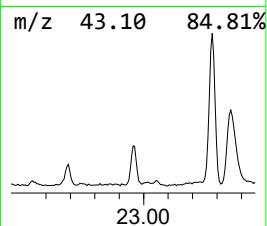
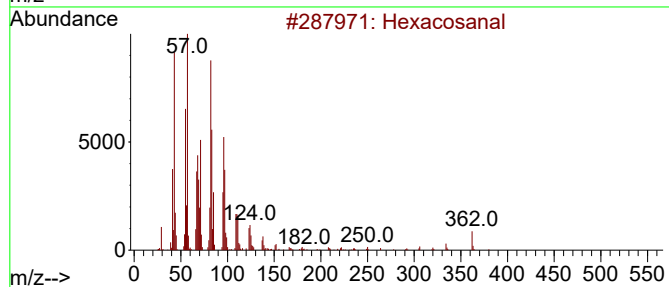
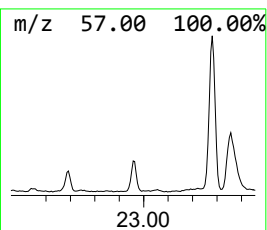
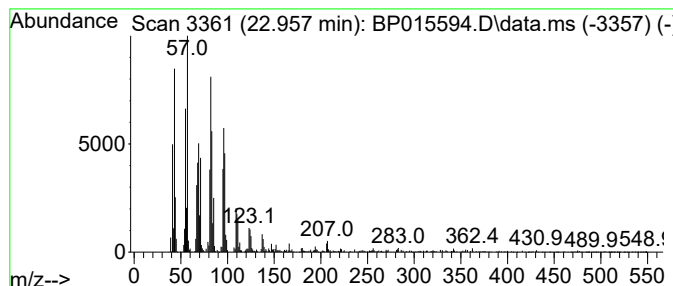
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Hexacosanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.957	5.59 ng/ul	598872	Perylene-d12	24.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosanal	380	C26H52O	026627-85-0	95
2			Octadecanal	268	C18H36O	000638-66-4	94
3			16-Octadecenal	266	C18H34O	056554-87-1	94
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
5			14-Octadecenal	266	C18H34O	056554-89-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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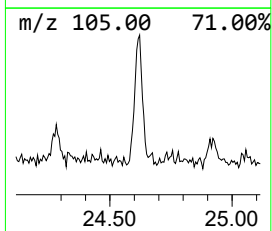
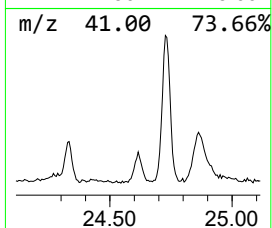
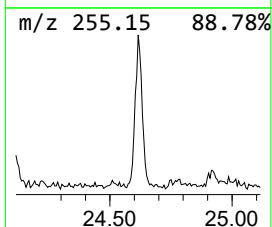
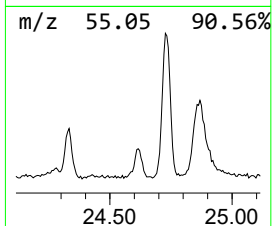
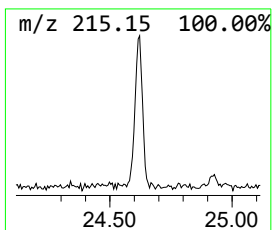
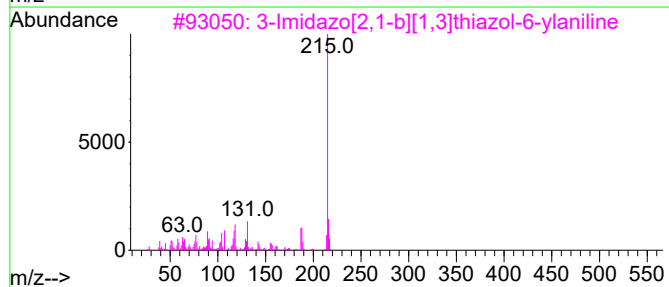
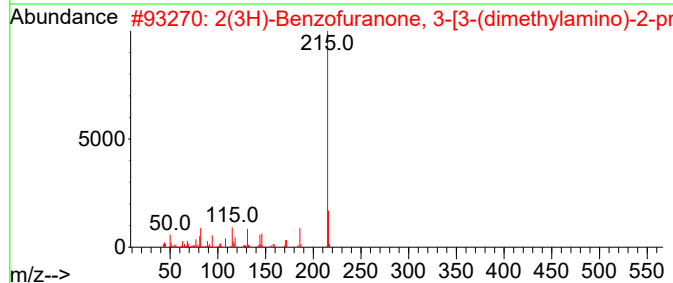
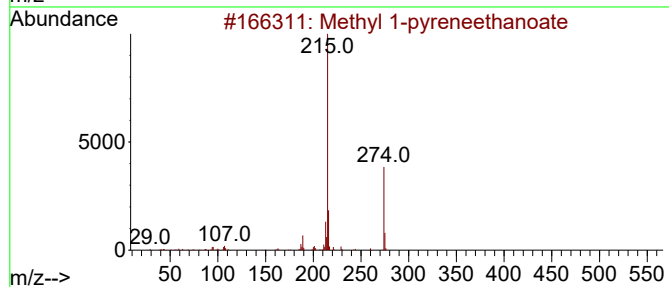
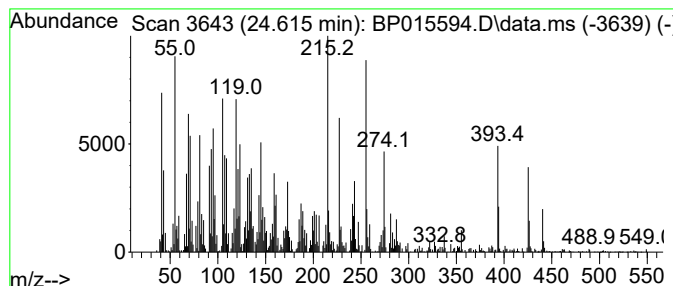
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.615	6.26 ng/ul	670503	Perylene-d12	24.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	30
2			2(3H)-Benzofuranone, 3-[3-(dimet...	215	C13H13NO2	056771-83-6	15
3			3-Imidazo[2,1-b][1,3]thiazol-6-y...	215	C11H9N3S	861206-26-0	15
4			Indanidine	215	C11H13N5	085392-79-6	15
5			.alpha.-Benzoylthioacetic acid a...	255	C15H13NOS	013196-40-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
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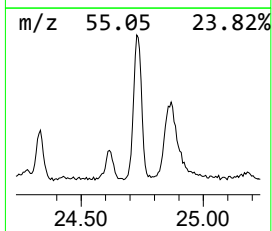
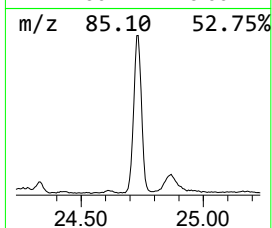
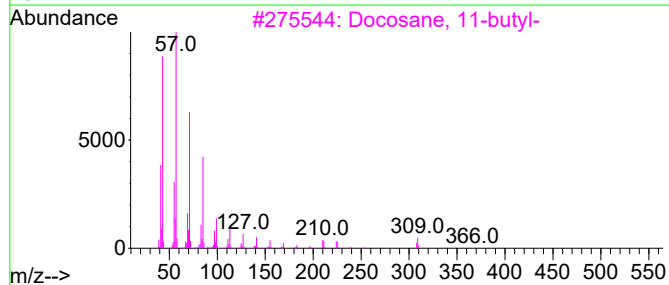
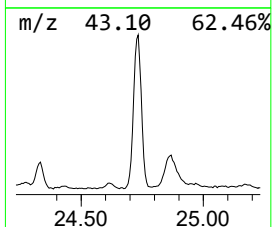
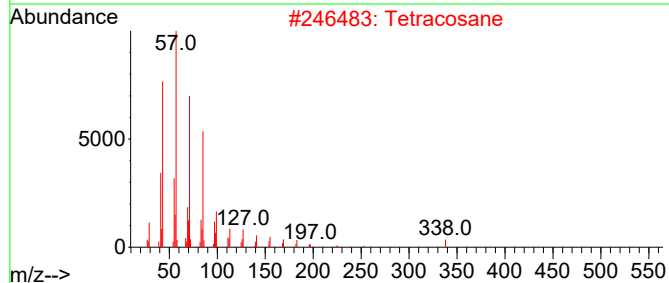
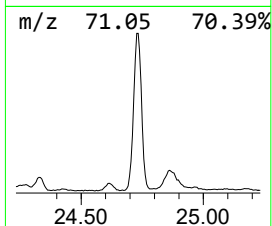
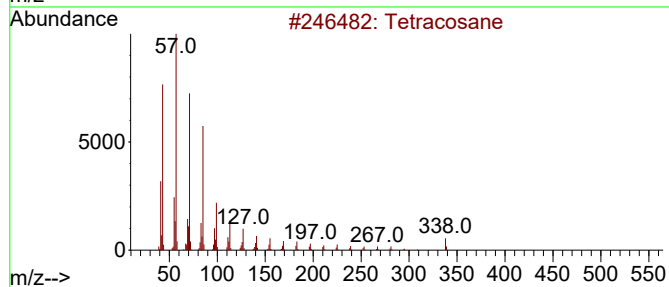
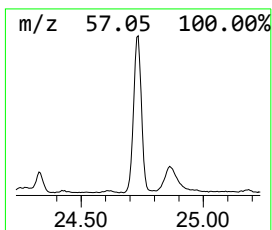
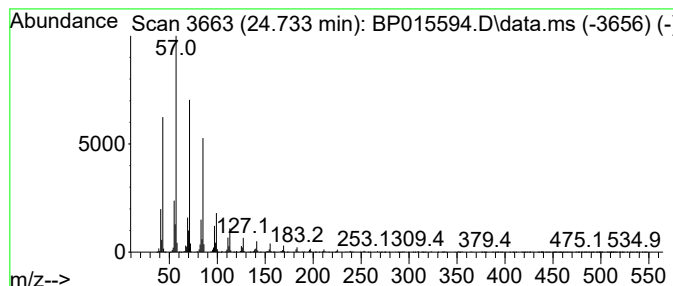
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.733	22.95 ng/ul	2458410	Perylene-d12		24.110	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetracosane		338	C24H50	000646-31-1	96
2	Tetracosane		338	C24H50	000646-31-1	94
3	Docosane, 11-butyl-		366	C26H54	013475-76-8	94
4	Heneicosane, 11-pentyl-		366	C26H54	014739-72-1	94
5	Docosane, 7-hexyl-		394	C28H58	055373-86-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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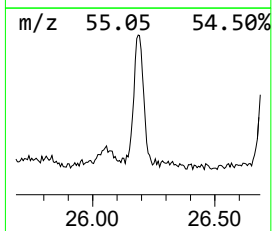
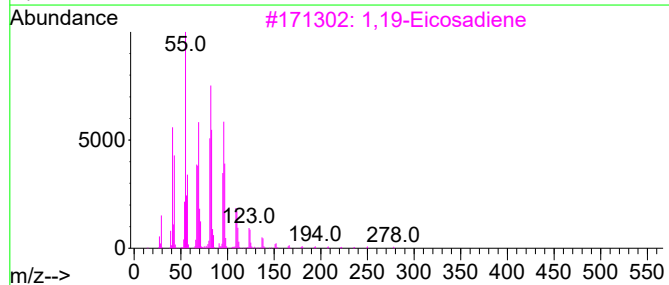
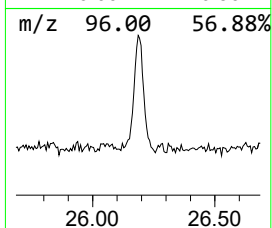
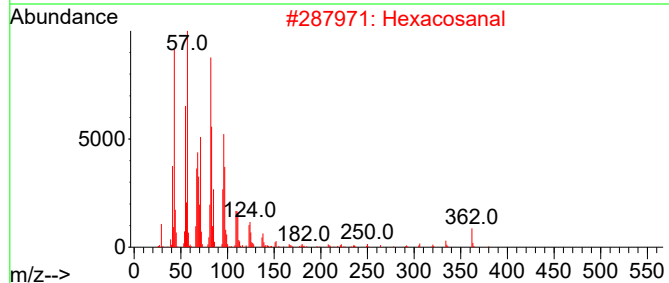
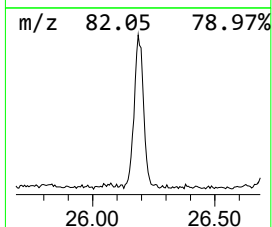
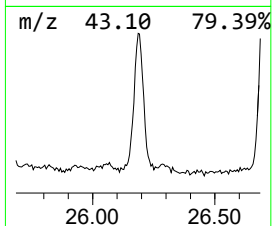
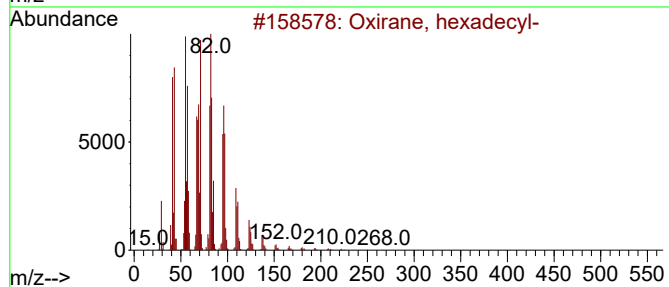
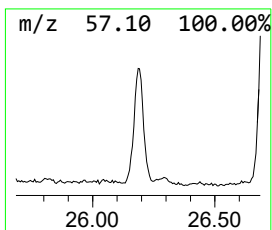
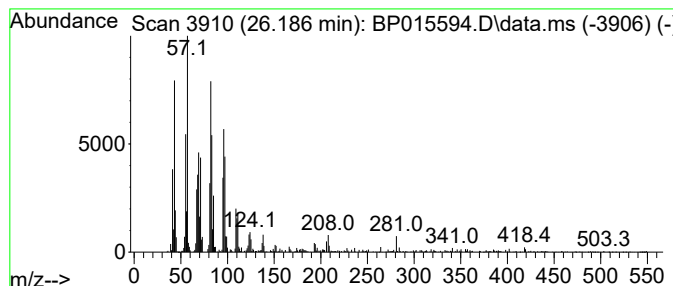
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.186	9.65 ng/ul	1033420	Perylene-d12	24.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91	
2	Hexacosanal		380	C26H52O	026627-85-0	91	
3	1,19-Eicosadiene		278	C20H38	014811-95-1	90	
4	Tetradecanal		212	C14H28O	000124-25-4	90	
5	Octacosanal		408	C28H56O	022725-64-0	90	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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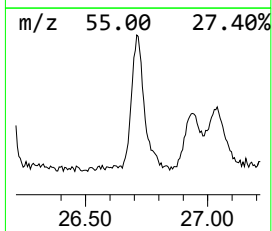
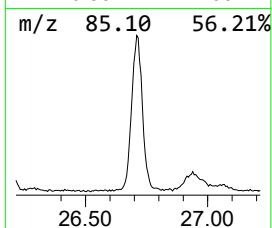
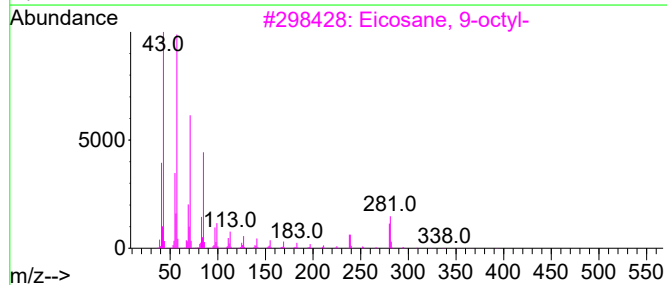
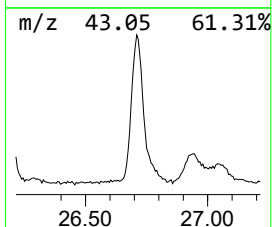
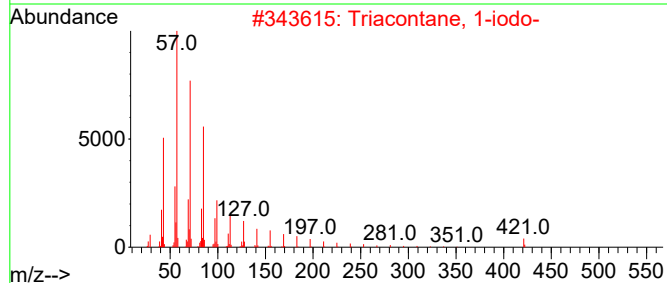
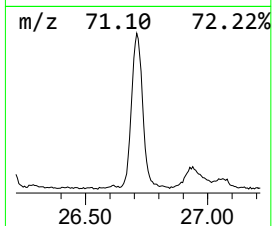
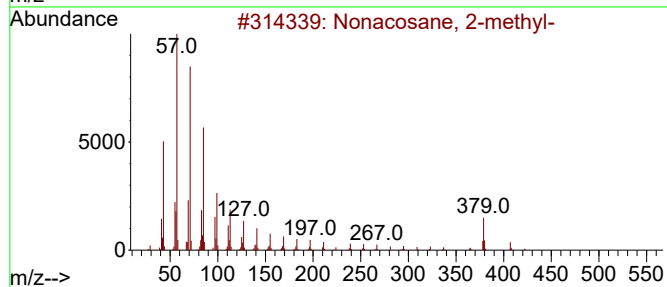
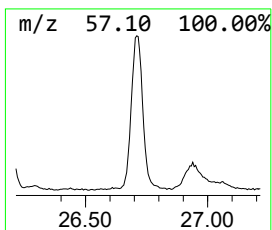
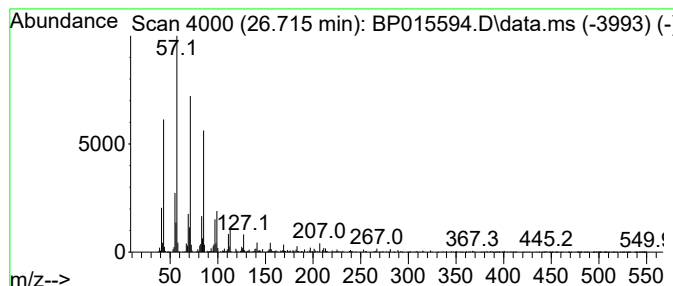
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.715	11.96 ng/ul	1280670	Perylene-d12	24.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosane, 2-methyl-	422	C30H62	001560-75-4	91
2			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91
3			Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015594.D
Acq On : 16 Jun 2023 23:07
Operator : MA/JU
Sample : 03080-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.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 ...	18.339	12.9	ng/ul	1368450	4	17.480	2124350	20.0
Octadecanoic acid	19.563	3.7	ng/ul	528274	5	21.563	2857240	20.0
(DEL) Alkane: S...	21.245	4.2	ng/ul	593649	5	21.563	2857240	20.0
Hexacosanal	22.957	5.6	ng/ul	598872	6	24.110	2142110	20.0
unknown-01	24.615	6.3	ng/ul	670503	6	24.110	2142110	20.0
(DEL) Alkane: S...	24.733	22.9	ng/ul	2458410	6	24.110	2142110	20.0
Oxirane, hexade...	26.186	9.7	ng/ul	1033420	6	24.110	2142110	20.0
(DEL) Alkane: S...	26.715	12.0	ng/ul	1280670	6	24.110	2142110	20.0