

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
 Data File : BP015900.D
 Acq On : 02 Jul 2023 00:26
 Operator : MA/JU
 Sample : 03242-22
 Misc :
 ALS Vial : 68 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCGC3

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-BP062623.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.375	29	32	38	rVB	33359	49104	1.38%	0.094%
2	3.899	117	121	122	rBV4	9267	13343	0.38%	0.026%
3	3.922	122	125	132	rVB	25101	39378	1.11%	0.075%
4	4.040	140	145	150	rVB2	44447	74201	2.09%	0.142%
5	4.140	160	162	168	rVB2	15409	21530	0.61%	0.041%
6	5.116	320	328	334	rBV2	71817	124880	3.52%	0.239%
7	5.422	377	380	381	rBV3	3363	3671	0.10%	0.007%
8	6.010	478	480	486	rVB6	3631	5007	0.14%	0.010%
9	6.087	489	493	495	rVV5	3416	3799	0.11%	0.007%
10	6.528	564	568	575	rBV8	7550	13499	0.38%	0.026%
11	6.693	588	596	602	rBV	49005	79702	2.25%	0.152%
12	6.999	644	648	654	rBV8	6812	13421	0.38%	0.026%
13	7.246	682	690	707	rBV	324743	943490	26.61%	1.805%
14	7.381	707	713	732	rVB	404439	827848	23.35%	1.584%
15	7.587	741	748	767	rBV	497175	995965	28.09%	1.905%
16	7.869	792	796	799	rVB6	3132	4368	0.12%	0.008%
17	8.052	819	827	841	rBV	833826	1653323	46.62%	3.163%
18	8.246	857	860	861	rBV3	6366	6453	0.18%	0.012%
19	8.546	908	911	912	rBV3	3237	4277	0.12%	0.008%
20	8.699	934	937	945	rBV10	3941	6877	0.19%	0.013%
21	8.804	948	955	969	rBV	253965	760658	21.45%	1.455%
22	8.910	969	973	986	rVB	55503	139147	3.92%	0.266%
23	9.246	1023	1030	1048	rBV	449770	1008765	28.45%	1.930%
24	9.393	1049	1055	1070	rVB7	22548	76645	2.16%	0.147%
25	9.575	1084	1086	1090	rVB4	5712	7853	0.22%	0.015%
26	9.634	1093	1096	1099	rVB5	3568	4767	0.13%	0.009%
27	9.769	1115	1119	1121	rBV5	4026	6194	0.17%	0.012%
28	9.869	1133	1136	1142	rVB8	3839	6841	0.19%	0.013%
29	9.975	1145	1154	1178	rBV	283966	852166	24.03%	1.630%
30	10.187	1183	1190	1199	rVB	12122	39077	1.10%	0.075%
31	10.275	1202	1205	1211	rBV8	7001	16496	0.47%	0.032%
32	10.387	1220	1224	1228	rVB7	3245	5868	0.17%	0.011%
33	10.557	1244	1253	1281	rBV	302034	1175423	33.15%	2.249%
34	10.881	1300	1308	1326	rBV	1167684	2477832	69.87%	4.740%
35	11.069	1334	1340	1360	rBV2	153275	560797	15.81%	1.073%
36	11.340	1384	1386	1389	rVB4	4042	4161	0.12%	0.008%

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37	11.863	1472	1475	1478	rBV5	3325	4681	0.13%	0.009%
38	12.081	1505	1512	1514	rBV8	8193	13417	0.38%	0.026%
39	12.104	1514	1516	1520	rVV4	3693	4537	0.13%	0.009%
40	12.151	1520	1524	1525	rVB3	3487	3840	0.11%	0.007%
41	12.216	1531	1535	1541	rBV8	11182	20395	0.58%	0.039%
42	12.287	1544	1547	1552	rVB7	3407	5515	0.16%	0.011%
43	12.410	1563	1568	1569	rBV5	3696	5218	0.15%	0.010%
44	12.498	1579	1583	1590	rVB8	8196	15975	0.45%	0.031%
45	12.622	1600	1604	1608	rBV7	5251	9197	0.26%	0.018%
46	12.775	1626	1630	1632	rBV5	3559	4476	0.13%	0.009%
47	12.816	1632	1637	1640	rBV7	3356	6435	0.18%	0.012%
48	13.051	1668	1677	1679	rBV9	7433	15480	0.44%	0.030%
49	13.292	1713	1718	1721	rBV6	4135	6345	0.18%	0.012%
50	13.428	1735	1741	1742	rBV6	7372	13141	0.37%	0.025%
51	13.451	1742	1745	1749	rVV6	10302	13353	0.38%	0.026%
52	13.504	1749	1754	1758	rVV8	5761	11112	0.31%	0.021%
53	13.575	1758	1766	1773	rVV5	26896	61277	1.73%	0.117%
54	13.675	1777	1783	1787	rBV5	20814	32551	0.92%	0.062%
55	13.728	1787	1792	1793	rVV5	6467	11074	0.31%	0.021%
56	13.757	1795	1797	1801	rVB5	3380	4015	0.11%	0.008%
57	13.998	1833	1838	1844	rBV9	29205	46017	1.30%	0.088%
58	14.110	1851	1857	1871	rBV	1057959	1911618	53.91%	3.657%
59	14.298	1885	1889	1891	rVB4	5817	8076	0.23%	0.015%
60	14.398	1899	1906	1921	rBV	1457036	2379024	67.09%	4.551%
61	14.569	1931	1935	1940	rVB7	10364	17090	0.48%	0.033%
62	14.634	1942	1946	1947	rBV4	4820	5545	0.16%	0.011%
63	14.698	1950	1957	1973	rBV	1929856	3242697	91.44%	6.204%
64	14.928	1993	1996	2000	rBV5	10123	13087	0.37%	0.025%
65	15.016	2005	2011	2024	rBV4	99651	406755	11.47%	0.778%
66	15.116	2025	2028	2034	rVB4	37184	63753	1.80%	0.122%
67	15.292	2056	2058	2061	rVB4	4987	5684	0.16%	0.011%
68	15.516	2093	2096	2100	rBV4	13345	18172	0.51%	0.035%
69	15.598	2105	2110	2116	rBV9	18098	33752	0.95%	0.065%
70	15.698	2119	2127	2144	rBV	1545153	2934434	82.75%	5.614%
71	15.886	2153	2159	2173	rBV3	118923	374402	10.56%	0.716%
72	16.069	2185	2190	2202	rBV	347688	586882	16.55%	1.123%
73	16.381	2240	2243	2245	rBV	17099	21416	0.60%	0.041%
74	16.551	2268	2272	2277	rBV7	20755	35277	0.99%	0.067%
75	16.628	2281	2285	2294	rVB	44972	78610	2.22%	0.150%
76	16.839	2317	2321	2330	rBV2	65208	123814	3.49%	0.237%

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77	17.175	2375	2378	2381	rBV5	20411	27465	0.77%	0.053%
78	17.333	2402	2405	2413	rBV7	33178	53781	1.52%	0.103%
79	17.463	2421	2427	2432	rBV	2143196	3255465	91.80%	6.228%
80	17.504	2432	2434	2439	rVV	370770	564253	15.91%	1.079%
81	17.569	2439	2445	2465	rVB2	1392869	2734688	77.12%	5.232%
82	18.163	2543	2546	2549	rBV2	30137	41937	1.18%	0.080%
83	18.204	2550	2553	2557	rBV2	84054	102383	2.89%	0.196%
84	18.257	2558	2562	2567	rBV	679907	913681	25.77%	1.748%
85	18.316	2567	2572	2581	rBV	2436940	3192290	90.02%	6.107%
86	19.404	2753	2757	2758	rBV2	141132	173052	4.88%	0.331%
87	19.427	2758	2761	2763	rVV2	286142	400807	11.30%	0.767%
88	19.469	2765	2768	2776	rVB	399198	629531	17.75%	1.204%
89	19.539	2776	2780	2787	rBV	655568	957737	27.01%	1.832%
90	19.792	2818	2823	2836	rBV2	1783688	3012862	84.96%	5.764%
91	20.204	2891	2893	2897	rBV	127162	144622	4.08%	0.277%
92	20.263	2901	2903	2907	rVB	199137	194359	5.48%	0.372%
93	21.221	3063	3066	3073	rVB	806779	1080328	30.46%	2.067%
94	21.551	3118	3122	3127	rBV	1432067	1989657	56.11%	3.806%
95	23.227	3403	3407	3413	rVB	1120119	1728005	48.73%	3.306%
96	24.098	3550	3555	3572	rVB	1169361	2932506	82.70%	5.610%
97	24.657	3645	3650	3660	rVB	1663799	3546141	100.00%	6.784%

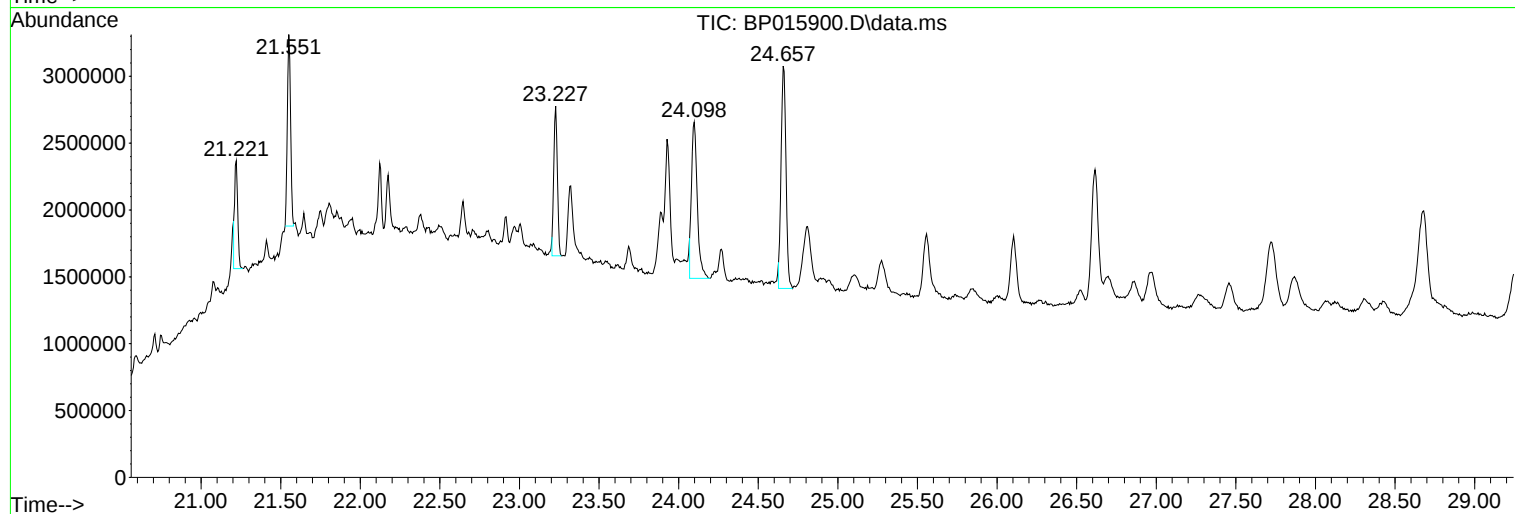
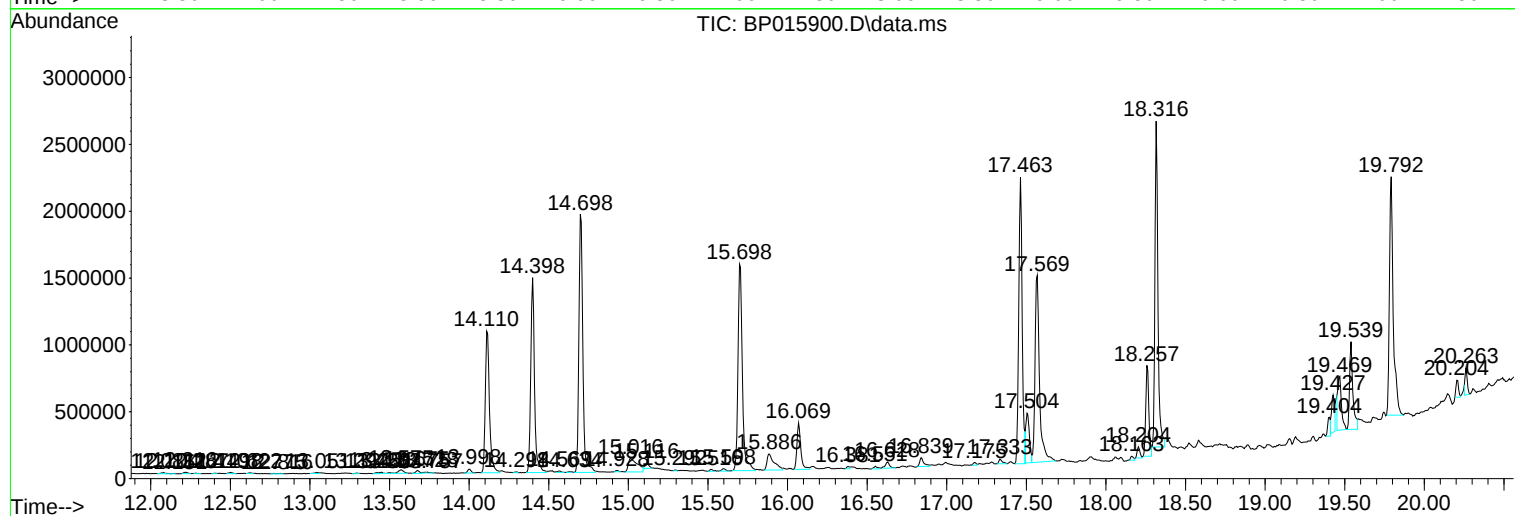
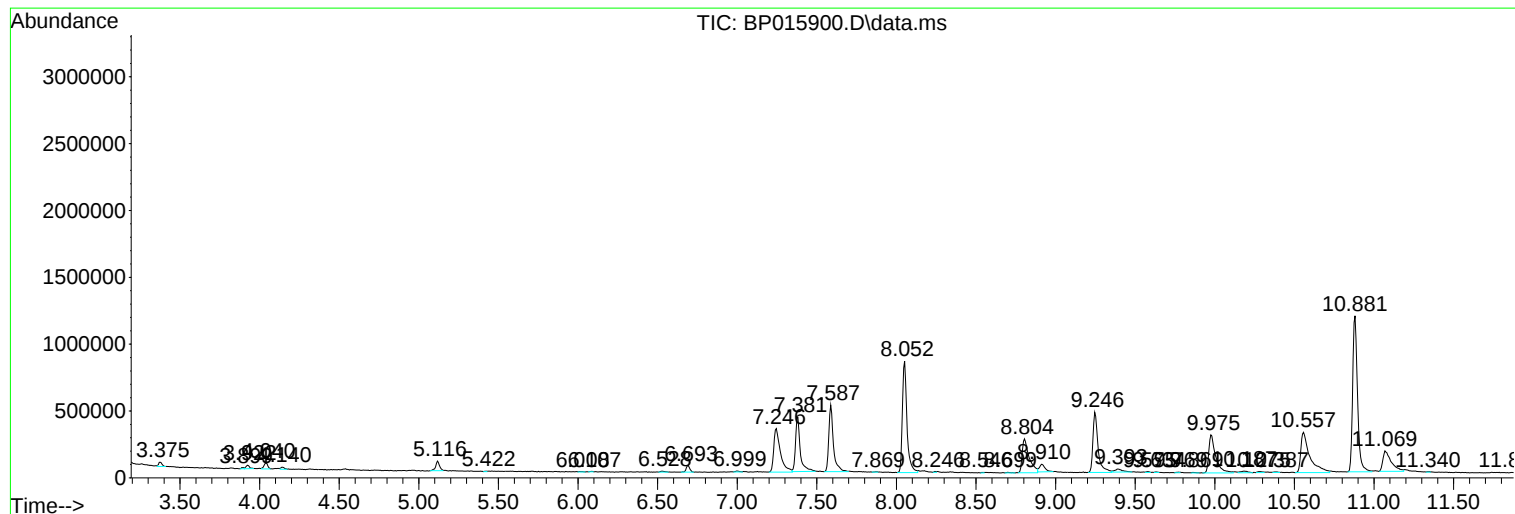
Sum of corrected areas: 52270515

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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



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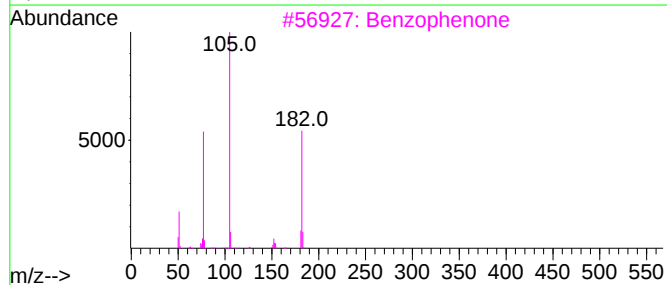
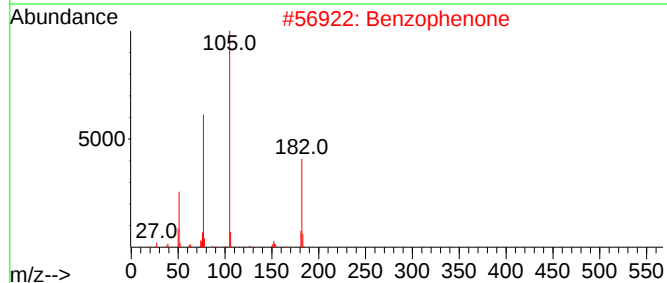
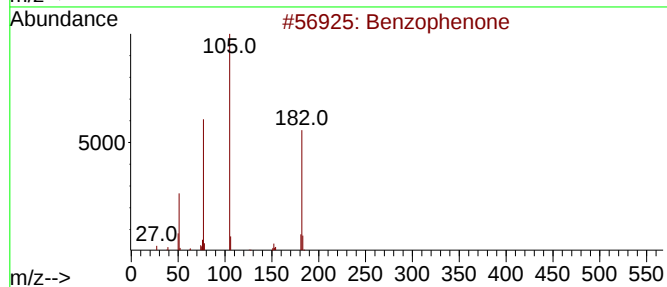
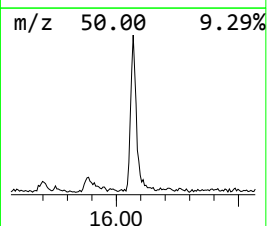
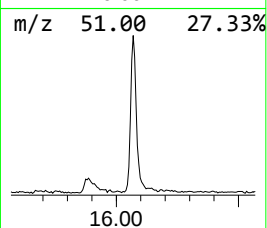
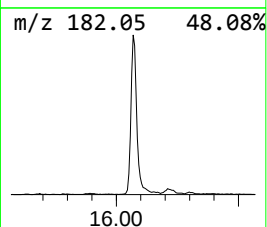
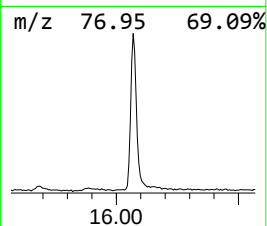
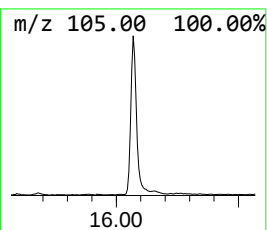
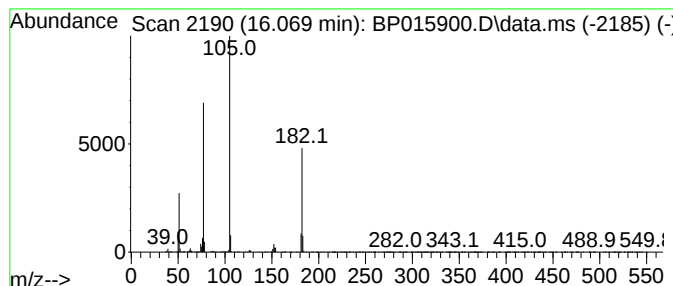
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.069	3.62 ng/ul	586882	Acenaphthene-d10	14.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Benzophenone	182	C13H10O	000119-61-9	91



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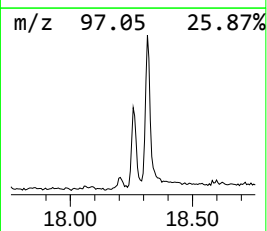
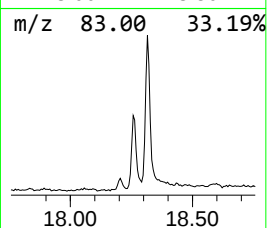
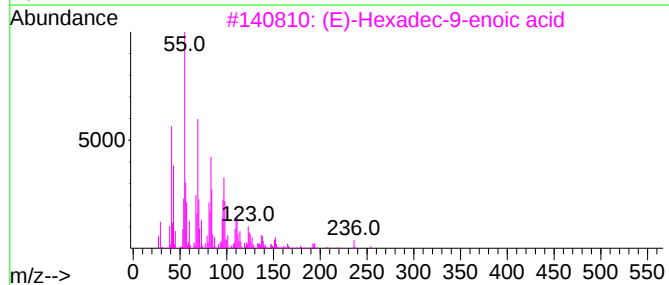
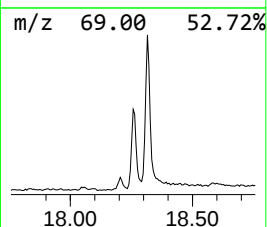
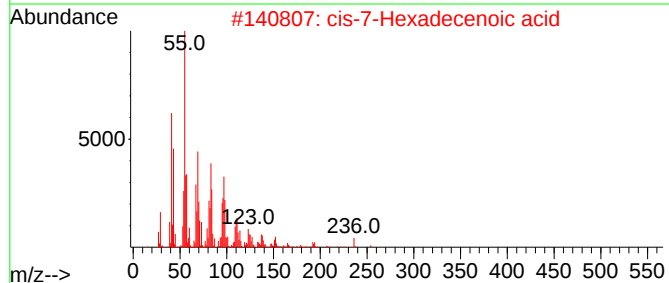
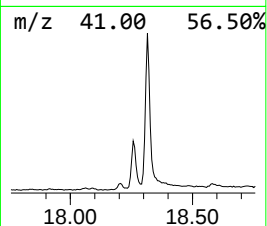
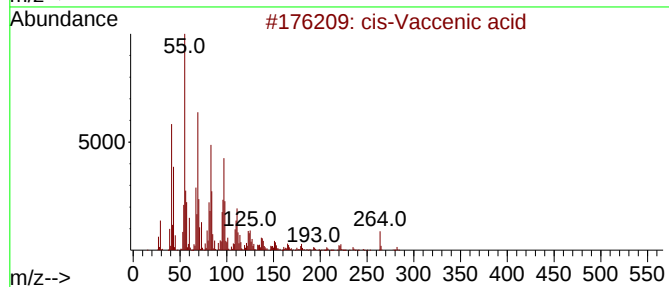
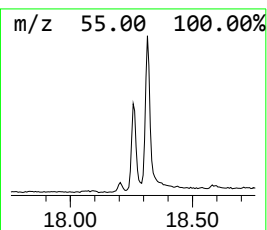
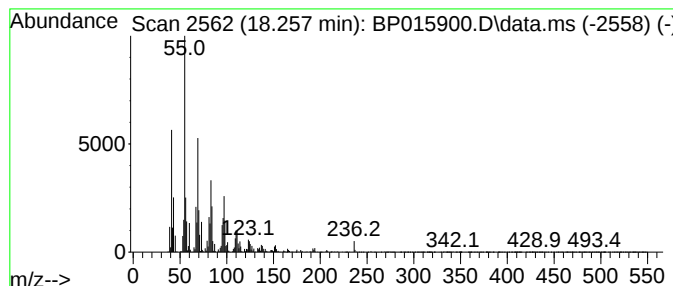
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 cis-Vaccenic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	5.61 ng/ul	913681	Phenanthrene-d10	17.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	91
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	91
4			cis-10-Nonadecenoic acid	296	C19H36O2	073033-09-7	91
5			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	91



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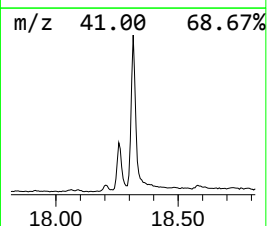
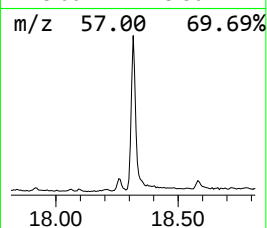
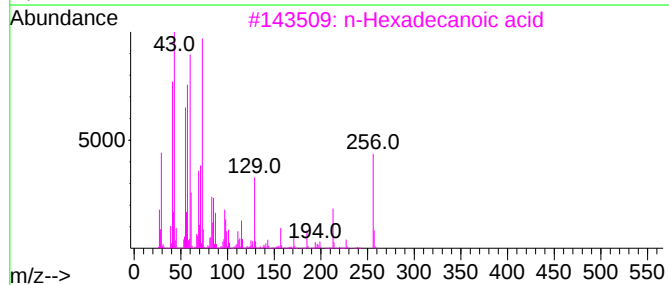
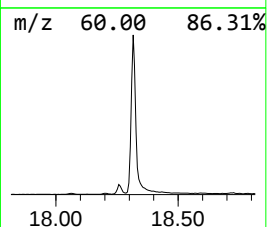
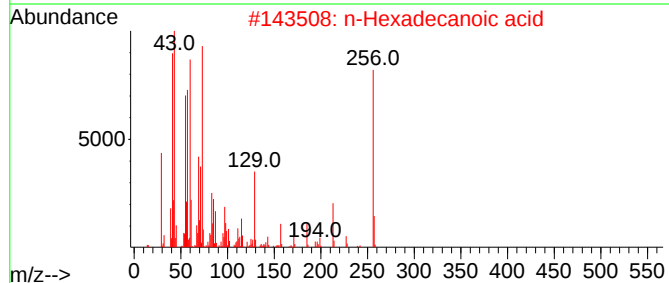
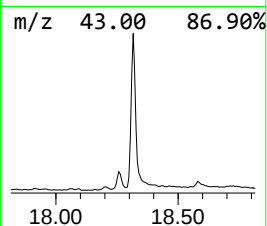
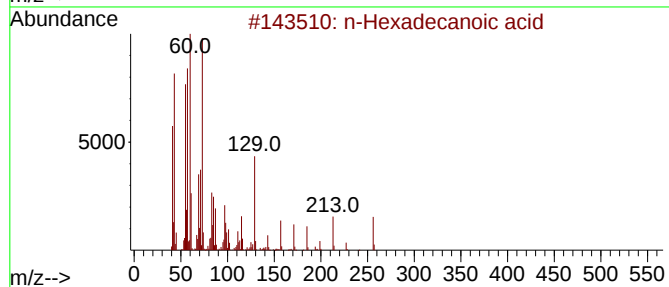
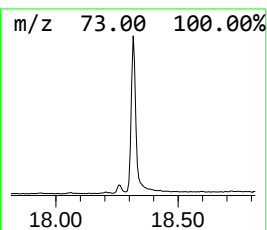
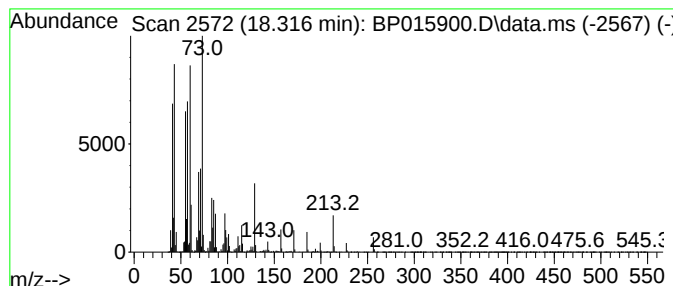
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.316	19.61 ng/ul	3192290	Phenanthrene-d10	17.463

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



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Acq On : 02 Jul 2023 00:26
Operator : MA/JU
Sample : 03242-22
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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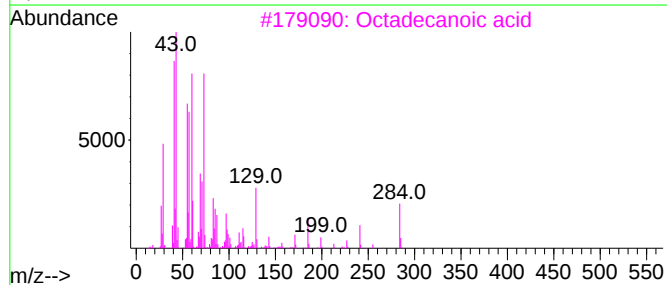
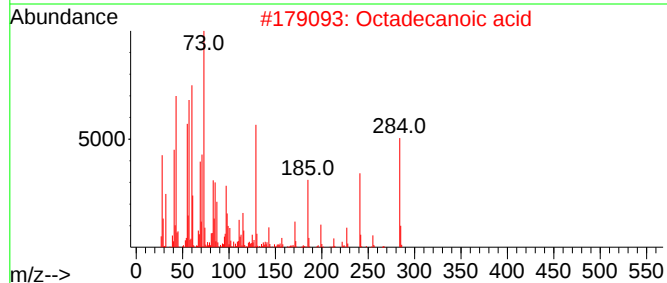
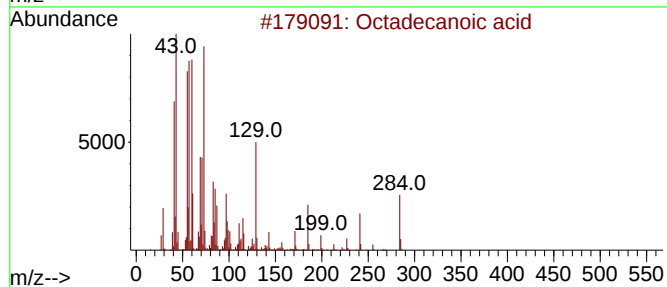
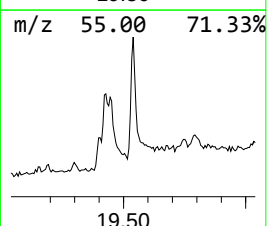
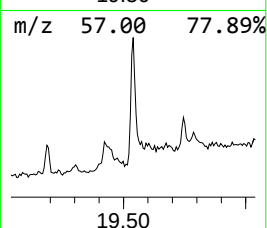
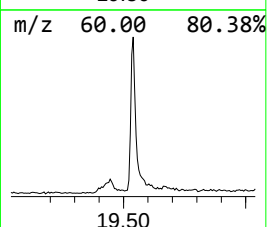
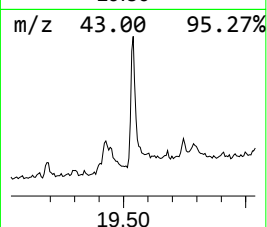
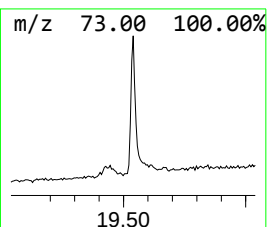
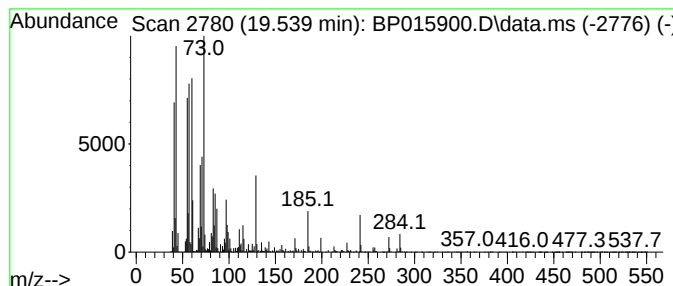
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.539	9.63 ng/ul	957737	Chrysene-d12	21.551

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	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	98
5			Octadecanoic acid	284	C18H36O2	000057-11-4	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015900.D
Acq On : 02 Jul 2023 00:26
Operator : MA/JU
Sample : 03242-22
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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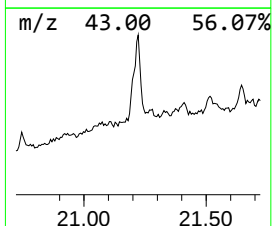
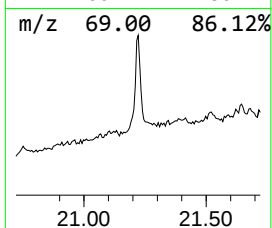
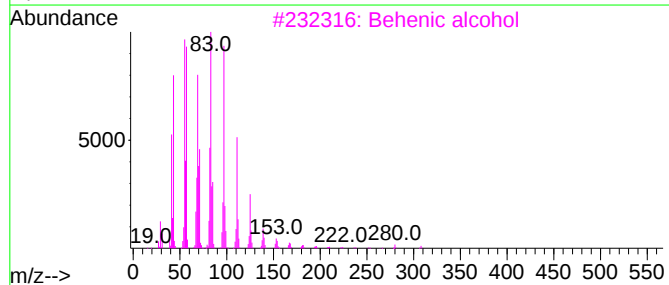
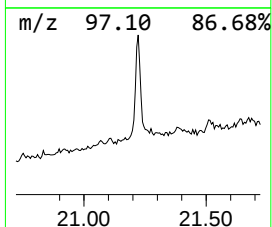
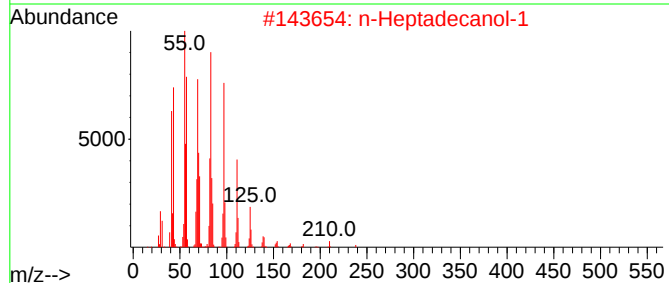
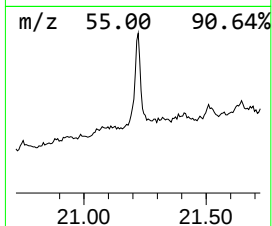
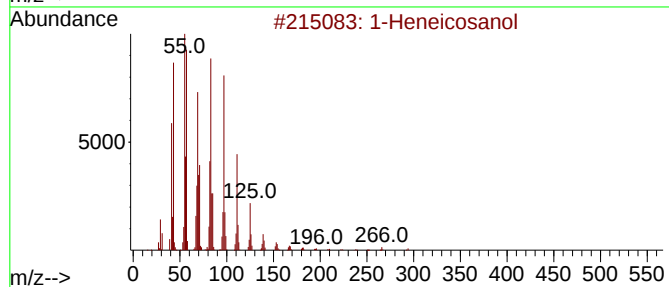
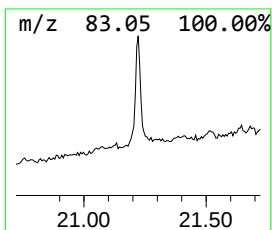
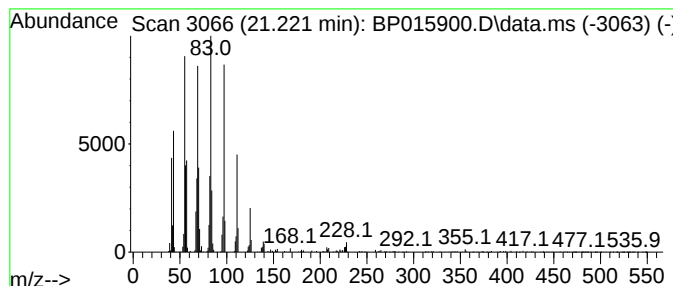
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	10.86 ng/ul	1080330	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3			Behenic alcohol	326	C22H46O	000661-19-8	90
4			1-Tricosene	322	C23H46	018835-32-0	90
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015900.D
Acq On : 02 Jul 2023 00:26
Operator : MA/JU
Sample : 03242-22
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGC3

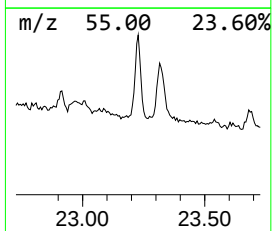
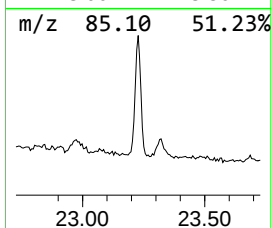
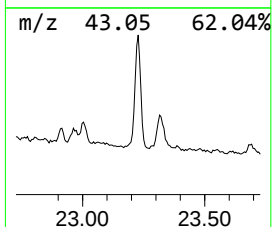
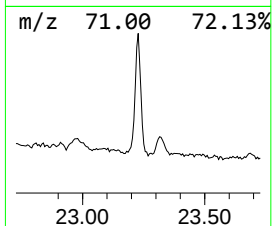
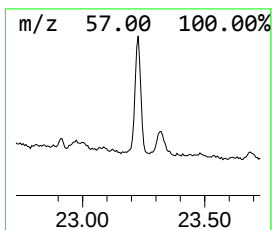
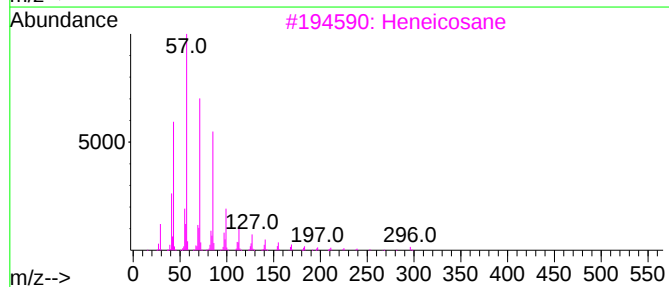
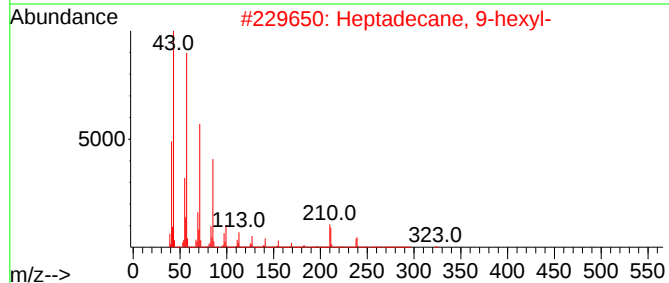
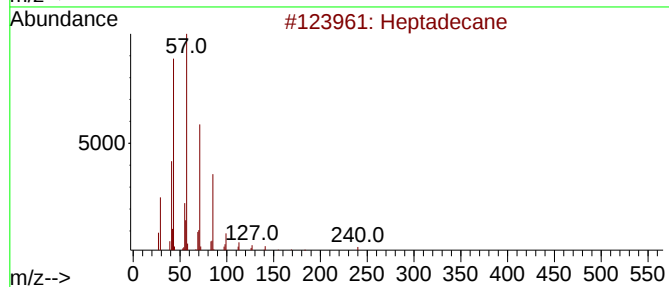
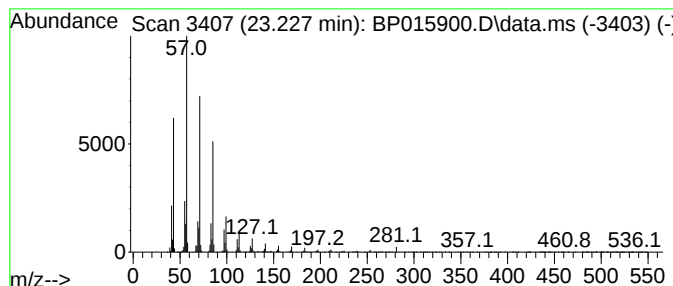
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.227	11.79 ng/ul	1728010	Perylene-d12	24.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015900.D
Acq On : 02 Jul 2023 00:26
Operator : MA/JU
Sample : 03242-22
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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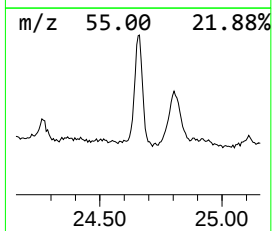
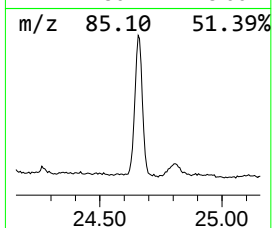
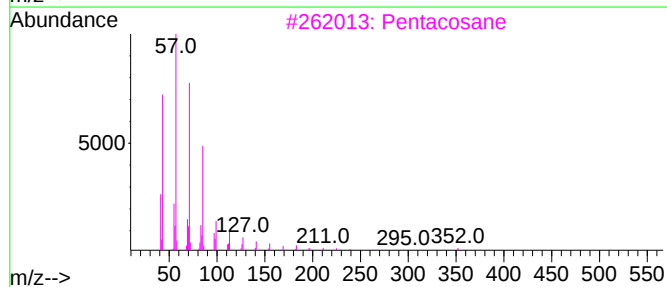
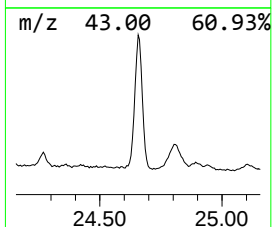
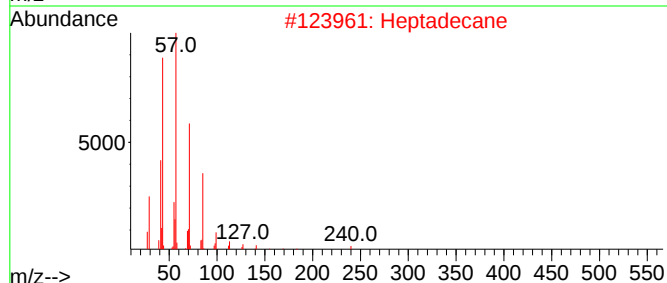
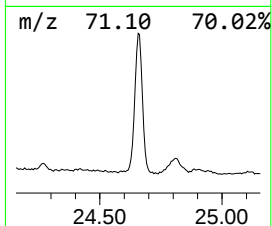
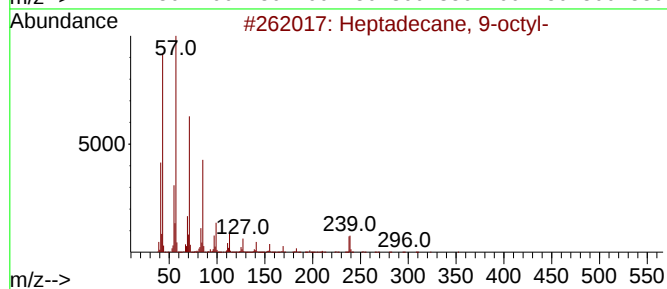
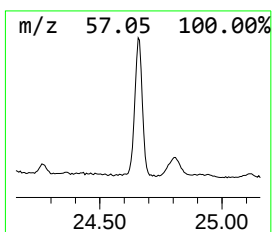
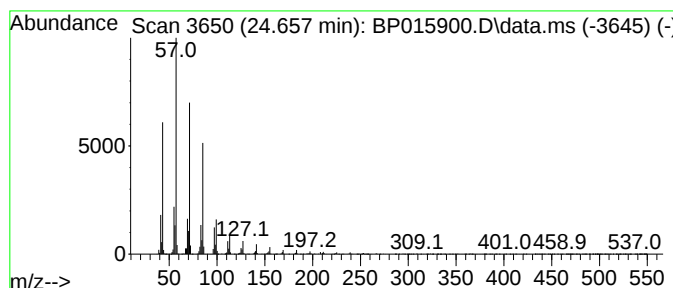
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.657	24.19 ng/ul	3546140	Perylene-d12	24.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2		Heptadecane	240	C17H36	000629-78-7	94
3		Pentacosane	352	C25H52	000629-99-2	94
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015900.D
Acq On : 02 Jul 2023 00:26
Operator : MA/JU
Sample : 03242-22
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGC3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.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
Benzophenone	16.069	3.6	ng/ul	586882	3	14.698	3242700	20.0
cis-Vaccenic acid	18.257	5.6	ng/ul	913681	4	17.463	3255470	20.0
n-Hexadecanoic ...	18.316	19.6	ng/ul	3192290	4	17.463	3255470	20.0
Octadecanoic acid	19.539	9.6	ng/ul	957737	5	21.551	1989660	20.0
1-Heneicosanol	21.221	10.9	ng/ul	1080330	5	21.551	1989660	20.0
(DEL) Alkane: S...	23.227	11.8	ng/ul	1728010	6	24.098	2932510	20.0
(DEL) Alkane: S...	24.657	24.2	ng/ul	3546140	6	24.098	2932510	20.0