

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP053123\
 Data File : BP015375.D
 Acq On : 01 Jun 2023 00:26
 Operator : CG/JU
 Sample : 02961-15
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 H0FQ5

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-BP051123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.417	35	39	47	rVB	33828	53542	0.88%	0.088%
2	3.864	112	115	129	rBV	101567	175960	2.88%	0.289%
3	3.964	130	132	136	rVB2	8843	10559	0.17%	0.017%
4	4.093	149	154	159	rVB3	7074	12885	0.21%	0.021%
5	4.193	168	171	178	rVB3	9835	13943	0.23%	0.023%
6	7.258	685	692	704	rBV	165974	281582	4.61%	0.462%
7	7.422	712	720	732	rBV	646031	1011924	16.57%	1.659%
8	7.628	748	755	766	rBV	632487	1040468	17.03%	1.706%
9	7.705	766	768	773	rVB6	4436	6548	0.11%	0.011%
10	8.105	827	836	844	rBV	655458	1053637	17.25%	1.728%
11	8.816	949	957	971	rBV	508694	874043	14.31%	1.433%
12	9.281	1028	1036	1050	rBV	858103	1435780	23.51%	2.354%
13	9.387	1050	1054	1058	rVV6	7039	13483	0.22%	0.022%
14	9.434	1058	1062	1073	rVB6	6080	13207	0.22%	0.022%
15	9.663	1097	1101	1107	rVB4	10695	18166	0.30%	0.030%
16	10.004	1152	1159	1171	rBV	718994	1229363	20.13%	2.016%
17	10.552	1242	1252	1267	rBV	921784	1682683	27.55%	2.759%
18	10.928	1309	1316	1324	rBV	958108	1620772	26.53%	2.658%
19	11.069	1333	1340	1356	rBV	560196	1025054	16.78%	1.681%
20	12.163	1521	1526	1531	rVB	9959	15973	0.26%	0.026%
21	12.246	1535	1540	1546	rVV10	2693	7556	0.12%	0.012%
22	12.328	1550	1554	1562	rVB9	6549	10759	0.18%	0.018%
23	12.516	1579	1586	1591	rBV	18099	31275	0.51%	0.051%
24	12.734	1617	1623	1628	rBV10	3814	7409	0.12%	0.012%
25	13.345	1723	1727	1730	rBV6	5685	7450	0.12%	0.012%
26	13.551	1757	1762	1766	rBV2	17001	25583	0.42%	0.042%
27	13.628	1770	1775	1783	rVB2	26887	42765	0.70%	0.070%
28	13.710	1785	1789	1797	rVB2	3247	8470	0.14%	0.014%
29	13.916	1817	1824	1825	rBV6	4061	7159	0.12%	0.012%
30	13.945	1825	1829	1835	rVB9	5873	11545	0.19%	0.019%
31	14.151	1854	1864	1871	rBV	2159403	3113478	50.97%	5.106%
32	14.263	1878	1883	1888	rVB6	13477	20352	0.33%	0.033%
33	14.322	1888	1893	1898	rBV	25962	37111	0.61%	0.061%
34	14.440	1906	1913	1928	rBV	2412564	3552335	58.16%	5.825%
35	14.622	1940	1944	1949	rVB	21106	28318	0.46%	0.046%
36	14.745	1958	1965	1971	rBV	1586602	2290390	37.50%	3.756%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051123.MA.M
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37	14.798	1971	1974	1980	rVV7	17327	37092	0.61%	0.061%
38	14.845	1980	1982	1989	rVV8	9945	14363	0.24%	0.024%
39	14.951	1993	2000	2016	rBV2	139418	315078	5.16%	0.517%
40	15.104	2023	2026	2029	rBV5	4575	7356	0.12%	0.012%
41	15.145	2029	2033	2038	rVB8	12089	17625	0.29%	0.029%
42	15.240	2046	2049	2055	rVB8	6145	11453	0.19%	0.019%
43	15.363	2067	2070	2077	rVB8	3539	7052	0.12%	0.012%
44	15.475	2083	2089	2094	rBV	76273	110893	1.82%	0.182%
45	15.569	2102	2105	2109	rVB2	24752	29904	0.49%	0.049%
46	15.739	2127	2134	2148	rBV	3059838	4477656	73.31%	7.343%
47	15.857	2148	2154	2167	rVV	1229319	1759719	28.81%	2.886%
48	15.975	2170	2174	2180	rVB3	24199	39261	0.64%	0.064%
49	16.098	2189	2195	2208	rVV	975239	1297814	21.25%	2.128%
50	16.192	2209	2211	2215	rVB5	7638	8346	0.14%	0.014%
51	16.434	2248	2252	2255	rBV	31369	46021	0.75%	0.075%
52	16.663	2286	2291	2297	rBV	242559	331486	5.43%	0.544%
53	16.798	2308	2314	2317	rBV	18778	32645	0.53%	0.054%
54	16.881	2325	2328	2335	rVB7	10665	19773	0.32%	0.032%
55	16.939	2336	2338	2342	rVB5	6224	6891	0.11%	0.011%
56	17.169	2375	2377	2384	rVB7	9464	13839	0.23%	0.023%
57	17.233	2384	2388	2391	rVV	27179	34154	0.56%	0.056%
58	17.286	2393	2397	2400	rVV4	22051	36829	0.60%	0.060%
59	17.322	2400	2403	2409	rVB	30562	42392	0.69%	0.070%
60	17.392	2409	2415	2419	rBV9	9757	21373	0.35%	0.035%
61	17.498	2427	2433	2441	rBV	1997769	2920425	47.81%	4.789%
62	17.598	2444	2450	2465	rVB2	3428530	4975222	81.45%	8.159%
63	17.769	2476	2479	2485	rBV5	12711	21607	0.35%	0.035%
64	17.969	2510	2513	2519	rBV2	21365	29539	0.48%	0.048%
65	18.139	2539	2542	2546	rVB	36399	43834	0.72%	0.072%
66	18.192	2549	2551	2554	rVV3	8723	9640	0.16%	0.016%
67	18.233	2556	2558	2567	rVB10	13697	27292	0.45%	0.045%
68	18.357	2574	2579	2587	rBV	385847	543233	8.89%	0.891%
69	18.633	2623	2626	2628	rBV2	24554	29289	0.48%	0.048%
70	19.175	2715	2718	2724	rVB2	81710	95729	1.57%	0.157%
71	19.233	2725	2728	2731	rVV3	87988	104056	1.70%	0.171%
72	19.263	2731	2733	2740	rVB3	57492	68314	1.12%	0.112%
73	19.398	2752	2756	2761	rVB3	61375	78455	1.28%	0.129%
74	19.469	2764	2768	2775	rVB	78650	114265	1.87%	0.187%
75	19.580	2783	2787	2795	rBV	140824	208043	3.41%	0.341%
76	19.822	2821	2828	2835	rBV	4639059	6108251	100.00%	10.017%

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 Title : SVOA CALIBRATION

77	20.310	2909	2911	2915	rVB	61614	60889	1.00%	0.100%
78	20.792	2990	2993	2997	rBV2	86846	98214	1.61%	0.161%
79	21.257	3067	3072	3081	rBV	707860	1227608	20.10%	2.013%
80	21.574	3121	3126	3133	rBV	2277291	3144314	51.48%	5.156%
81	21.698	3145	3147	3152	rVB2	76049	79961	1.31%	0.131%
82	22.480	3275	3280	3288	rVB	1390435	1978912	32.40%	3.245%
83	22.710	3316	3319	3326	rVB2	128480	176463	2.89%	0.289%
84	22.863	3341	3345	3353	rVB	233455	354465	5.80%	0.581%
85	23.963	3524	3532	3544	rVB2	2894843	5960198	97.58%	9.774%
86	24.127	3553	3560	3570	rVB	1403327	3012619	49.32%	4.940%

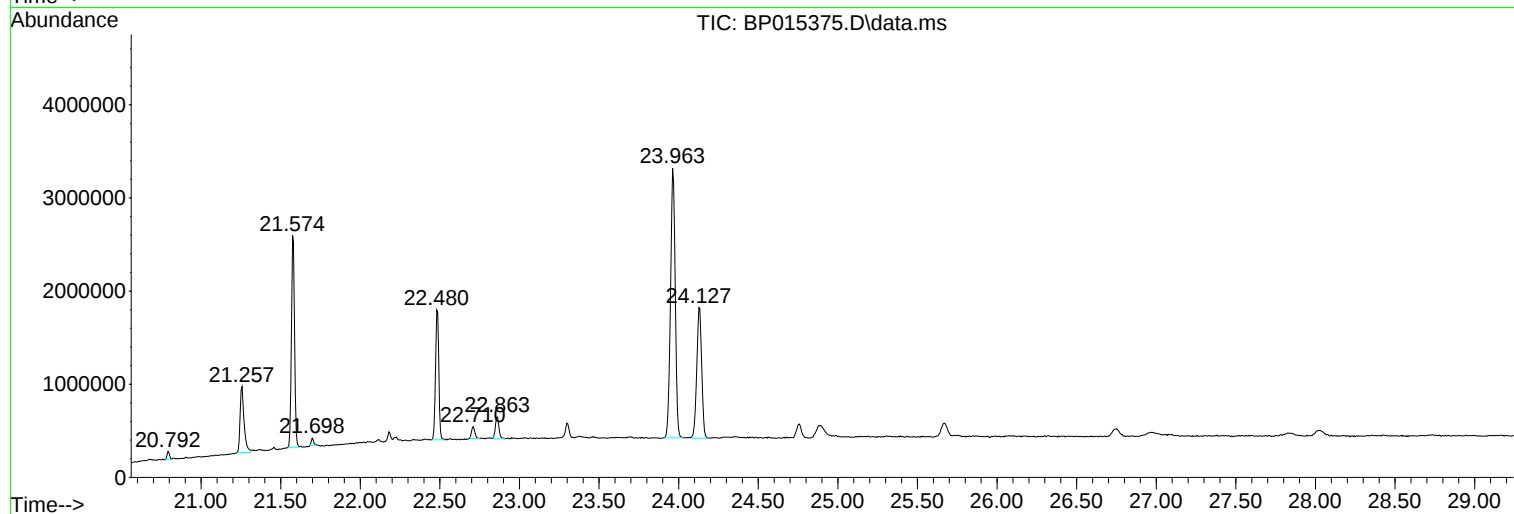
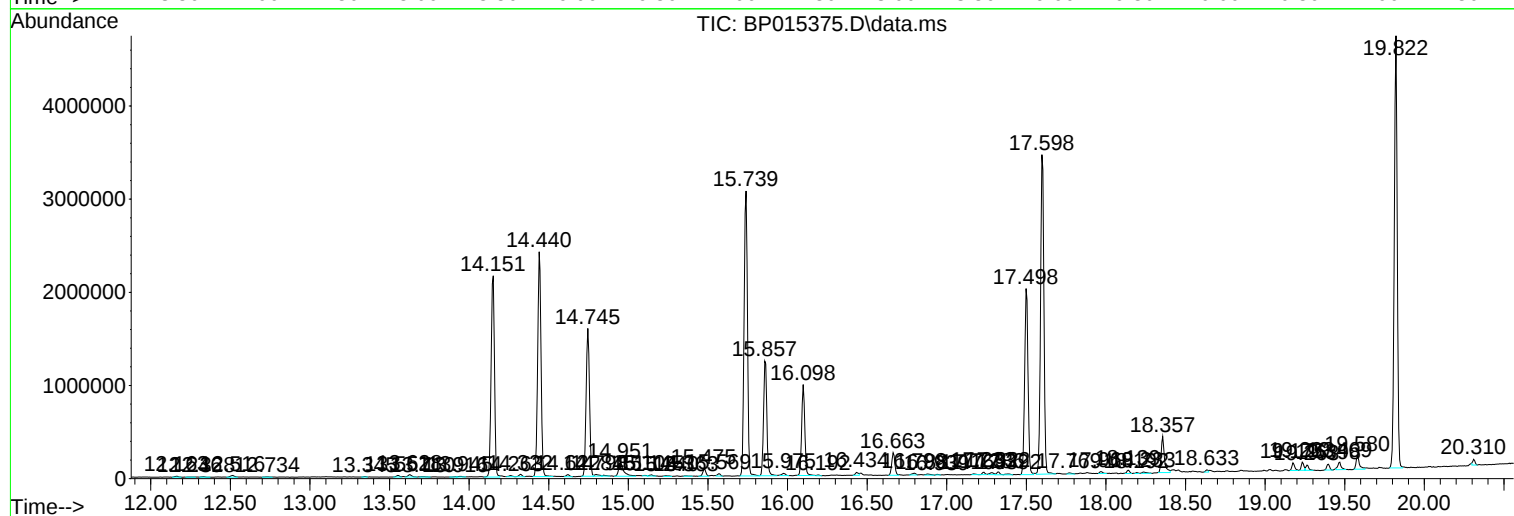
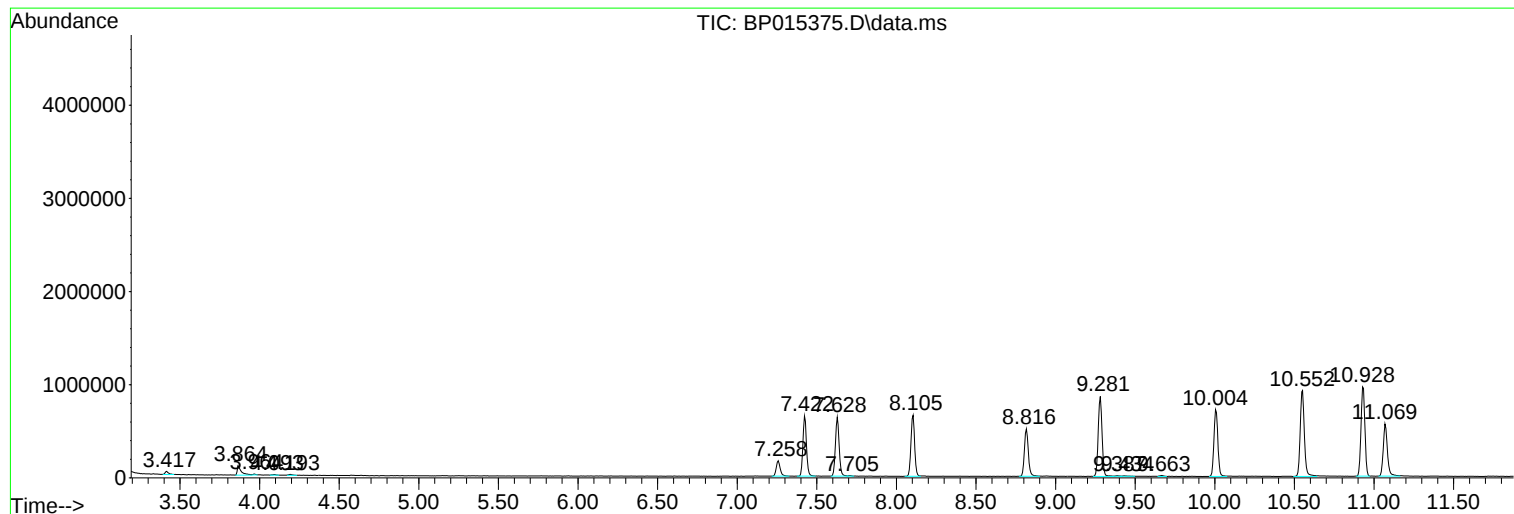
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051123.MA.M
Quant Title : SVOA CALIBRATION

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



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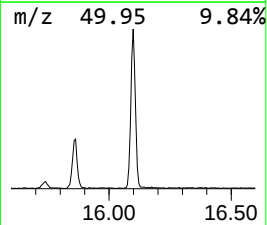
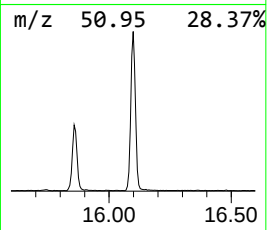
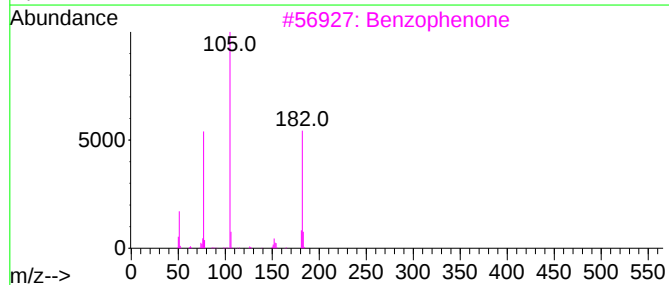
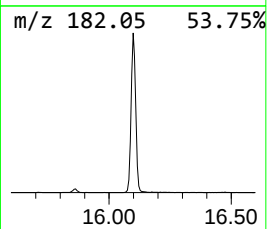
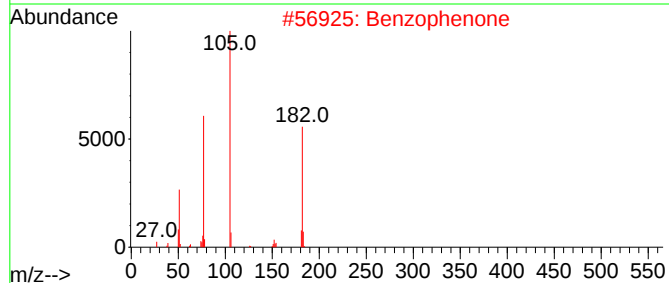
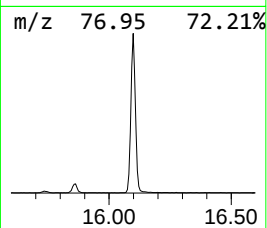
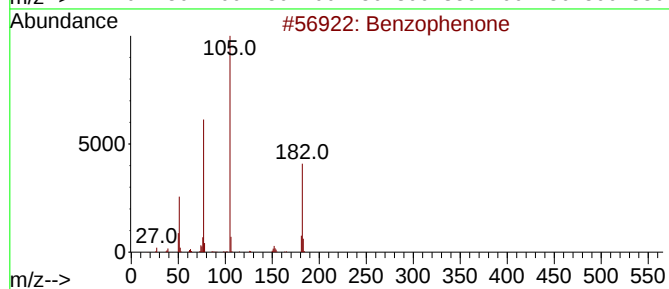
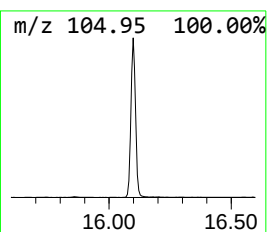
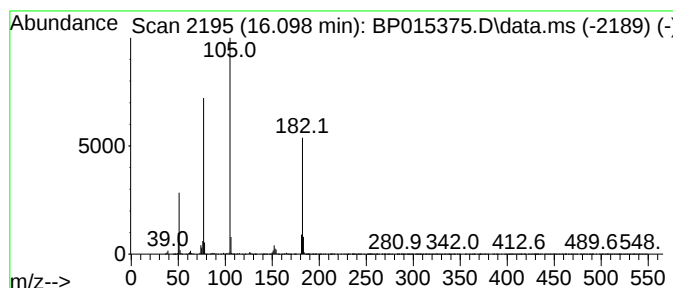
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	11.33 ng/ul	1297810	Acenaphthene-d10	14.745

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	78



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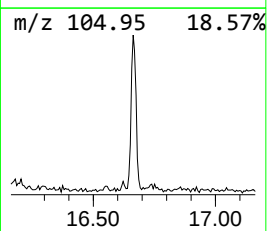
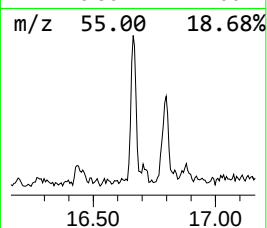
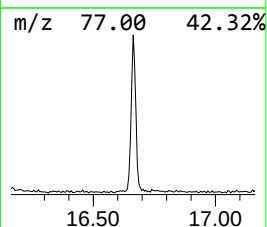
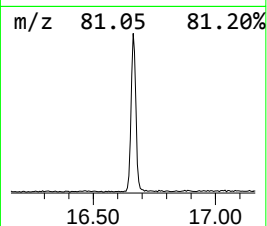
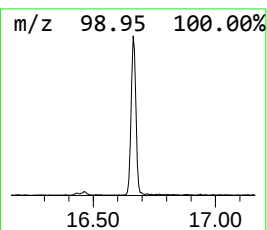
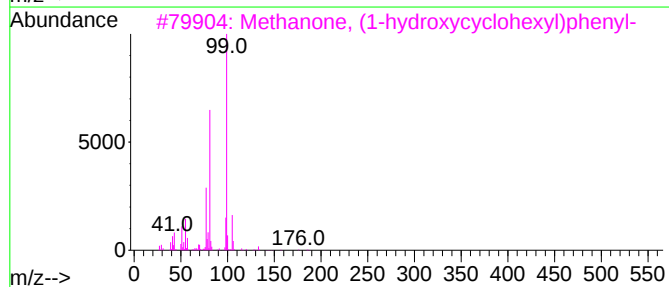
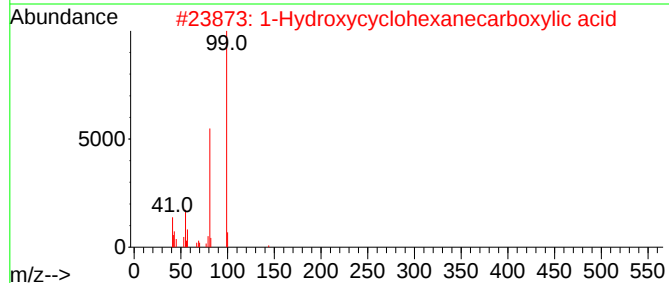
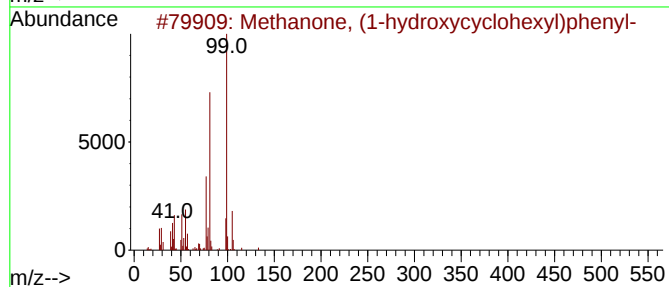
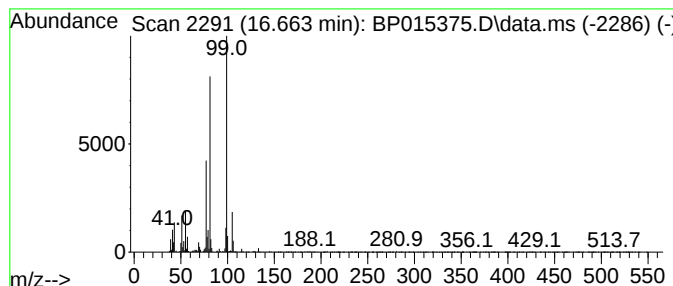
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Methanone, (1-hydroxycyclohexyl) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.663	2.27 ng/ul	331486	Phenanthrene-d10	17.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	86
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	53
3			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	49
4			1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	33
5			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	33



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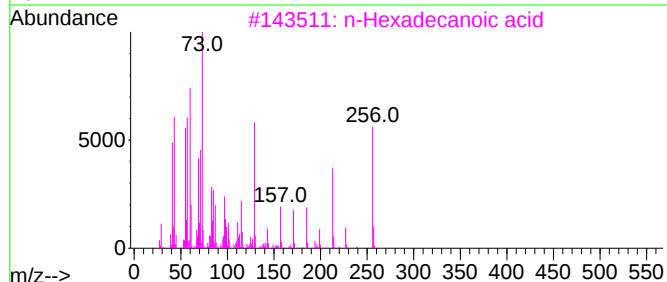
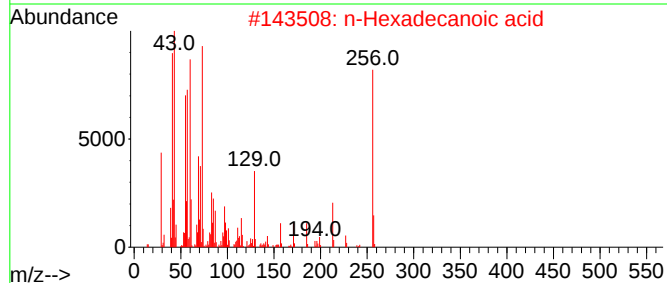
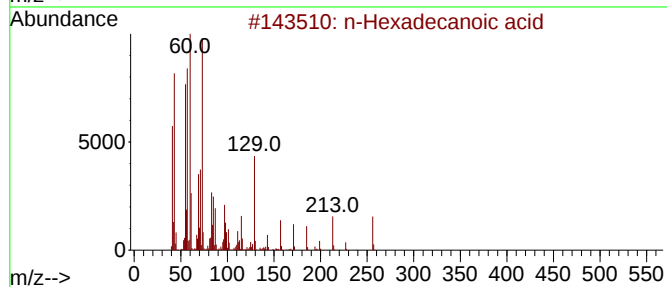
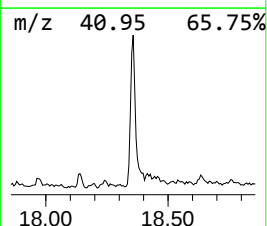
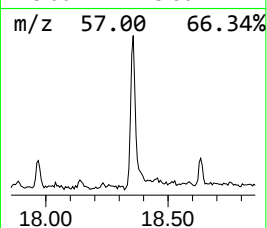
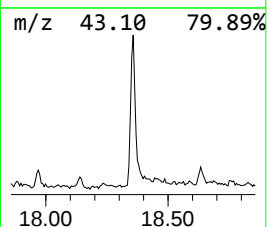
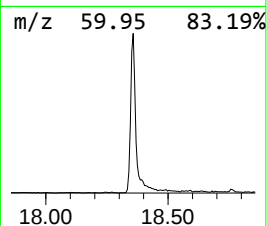
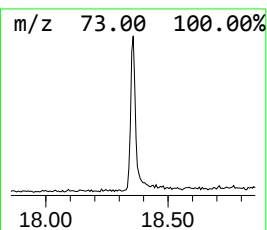
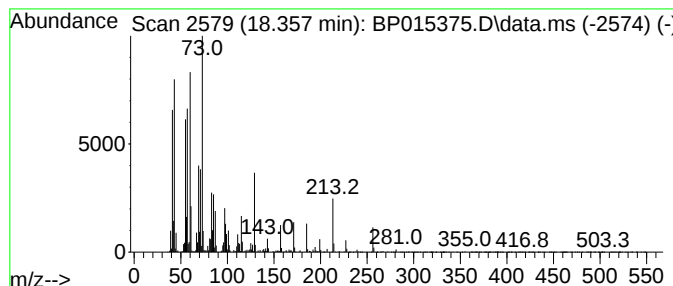
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.357	3.72 ng/ul	543233	Phenanthrene-d10	17.498

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	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Tridecanoic acid	214	C13H26O2	000638-53-9	97



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H0FQ5

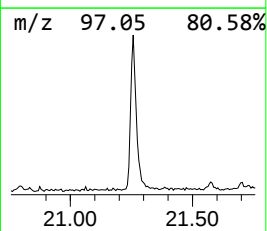
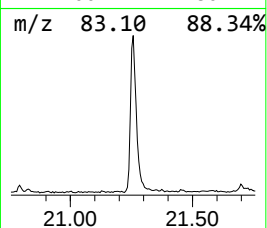
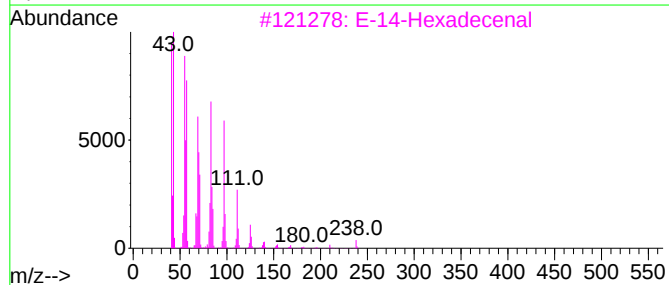
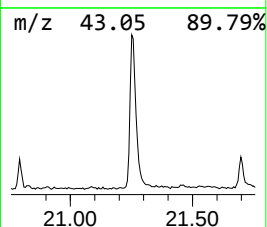
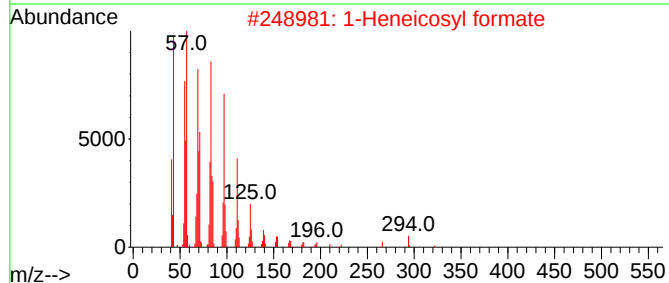
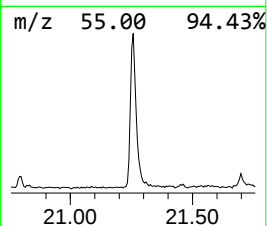
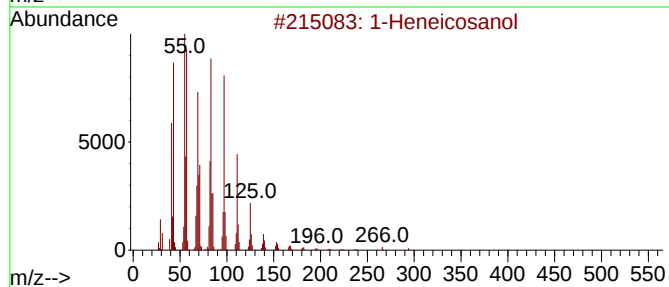
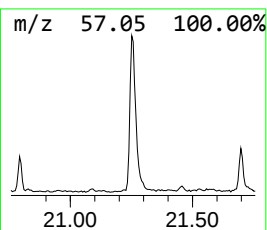
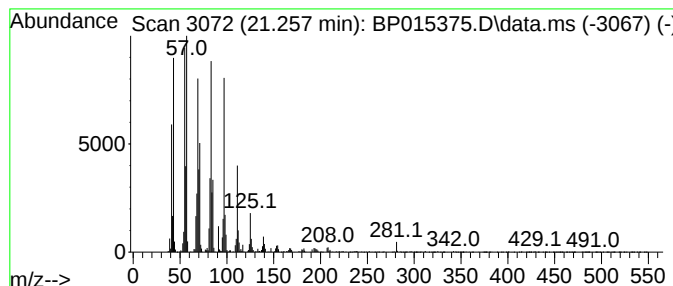
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	7.81 ng/ul	1227610	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			E-14-Hexadecenal	238	C16H30O	330207-53-9	94
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP053123\
Data File : BP015375.D
Acq On : 01 Jun 2023 00:26
Operator : CG/JU
Sample : 02961-15
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0FQ5

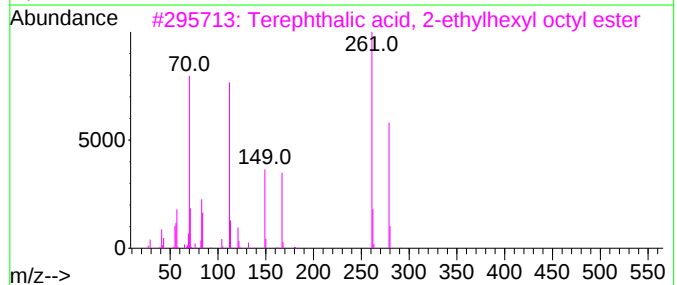
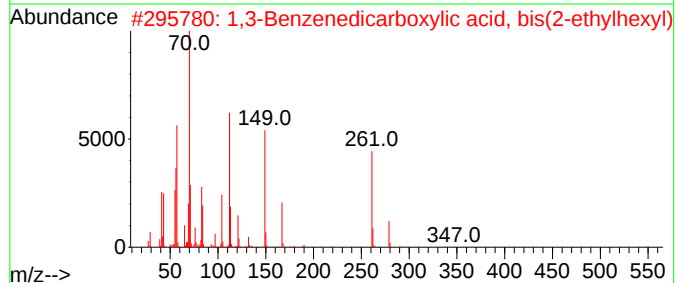
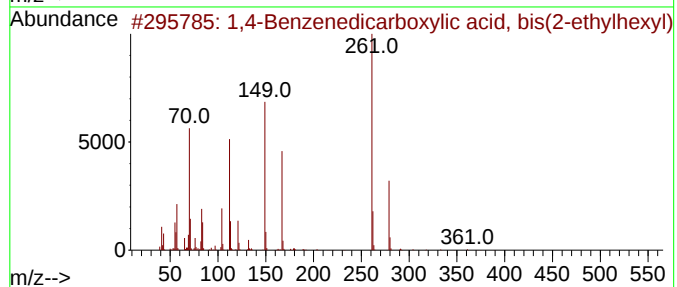
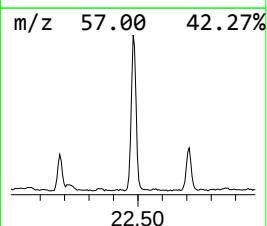
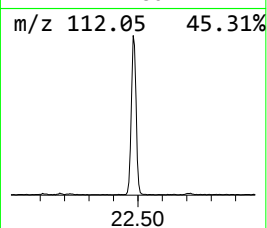
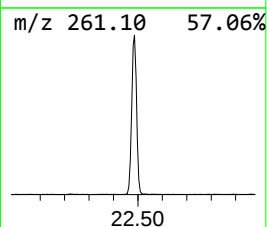
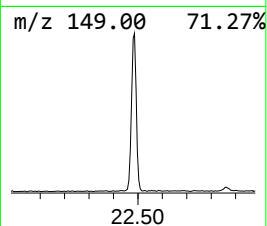
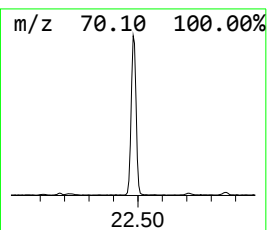
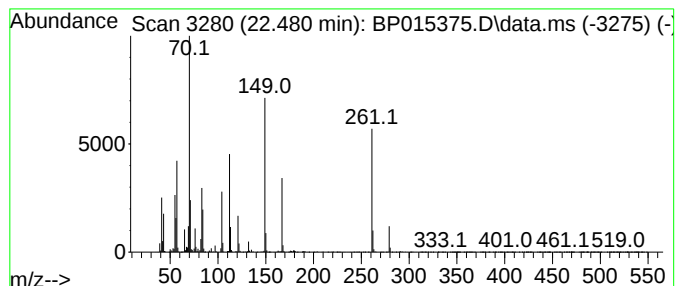
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.480	12.59 ng/ul	1978910	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
5			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP053123\
Data File : BP015375.D
Acq On : 01 Jun 2023 00:26
Operator : CG/JU
Sample : 02961-15
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0FQ5

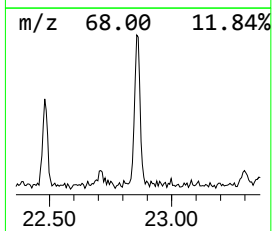
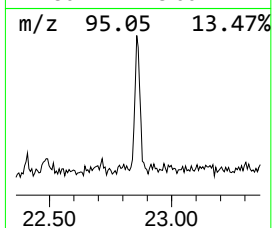
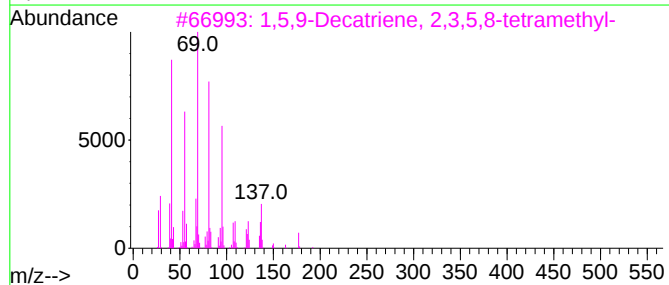
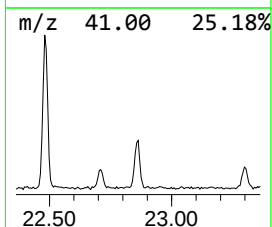
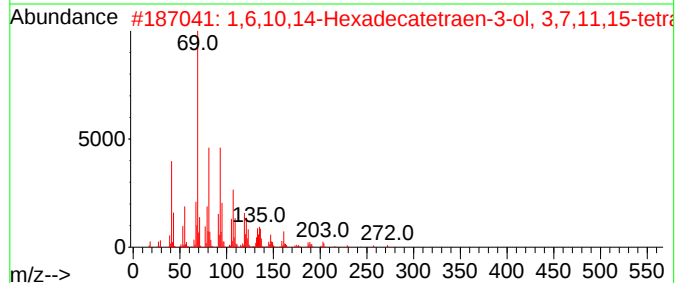
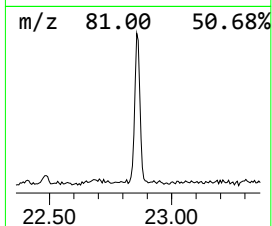
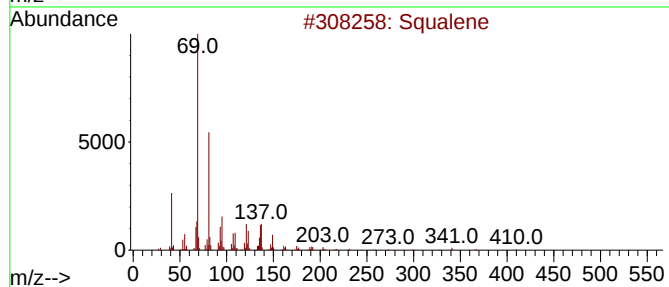
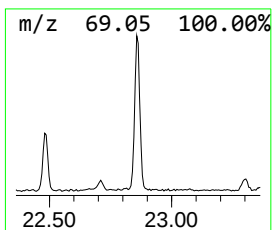
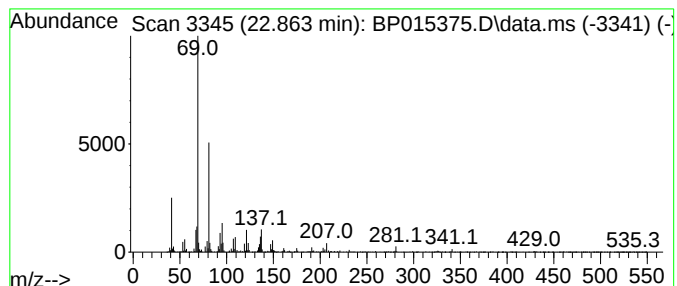
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.863	2.35 ng/ul	354465	Perylene-d12	24.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	72
2			1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	59
3			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	53
4			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53
5			Squalene	410	C30H50	000111-02-4	51



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP053123\
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Acq On : 01 Jun 2023 00:26
Operator : CG/JU
Sample : 02961-15
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0FQ5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051123.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	16.098	11.3	ng/ul	1297810	3	14.745	2290390	20.0
Methanone, (1-h...	16.663	2.3	ng/ul	331486	4	17.498	2920430	20.0
n-Hexadecanoic ...	18.357	3.7	ng/ul	543233	4	17.498	2920430	20.0
1-Heneicosanol	21.257	7.8	ng/ul	1227610	5	21.574	3144310	20.0
1,4-Benzenedica...	22.480	12.6	ng/ul	1978910	5	21.574	3144310	20.0
Squalene	22.863	2.4	ng/ul	354465	6	24.127	3012620	20.0