

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
 Data File : BP016153.D
 Acq On : 10 Jul 2023 11:52
 Operator : MA/JU
 Sample : 03356-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 YBW37

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: BP016153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.305	17	20	24	rBV3	34753	50947	0.55%	0.060%
2	3.346	24	27	39	rVB	79471	126954	1.37%	0.150%
3	3.793	100	103	125	rBV	699513	1429598	15.48%	1.687%
4	4.528	226	228	234	rVB3	14187	22402	0.24%	0.026%
5	7.210	677	684	701	rBV	607897	2001816	21.67%	2.362%
6	7.346	701	707	731	rVB	696387	1698285	18.38%	2.004%
7	7.552	736	742	775	rVB	879245	2115054	22.90%	2.495%
8	8.016	814	821	842	rBV	446220	1306935	14.15%	1.542%
9	8.763	940	948	987	rBV	777384	2814649	30.47%	3.321%
10	9.216	1017	1025	1055	rBV	759787	2202208	23.84%	2.598%
11	9.528	1073	1078	1082	rVB7	6736	11611	0.13%	0.014%
12	9.957	1143	1151	1175	rBV	505981	1909597	20.67%	2.253%
13	10.540	1241	1250	1271	rBV	499906	2361927	25.57%	2.787%
14	10.846	1295	1302	1326	rVB	800080	2008869	21.75%	2.370%
15	11.040	1328	1335	1370	rBV	524059	2501109	27.08%	2.951%
16	12.028	1498	1503	1509	rVB8	6893	14466	0.16%	0.017%
17	12.522	1580	1587	1593	rBV7	13281	36539	0.40%	0.043%
18	13.475	1746	1749	1756	rBV8	6409	12596	0.14%	0.015%
19	13.551	1756	1762	1771	rVV5	22852	53745	0.58%	0.063%
20	13.675	1778	1783	1788	rBV9	5942	10264	0.11%	0.012%
21	14.010	1833	1840	1844	rBV10	8386	19675	0.21%	0.023%
22	14.087	1846	1853	1882	rVV	2178047	4826187	52.24%	5.694%
23	14.304	1885	1890	1893	rVV2	13862	24998	0.27%	0.029%
24	14.363	1893	1900	1925	rVV2	3266705	5613966	60.77%	6.623%
25	14.545	1927	1931	1938	rVB4	18802	37601	0.41%	0.044%
26	14.669	1945	1952	1971	rBV	1611853	2778770	30.08%	3.278%
27	15.022	2006	2012	2040	rBV3	174954	1215012	13.15%	1.433%
28	15.439	2079	2083	2089	rVB9	10642	17479	0.19%	0.021%
29	15.486	2089	2091	2101	rVB6	15622	25254	0.27%	0.030%
30	15.675	2116	2123	2141	rBV	3296263	7095195	76.81%	8.371%
31	15.869	2150	2156	2180	rBV	373781	1601484	17.34%	1.889%
32	16.045	2180	2186	2205	rVB	1153068	1915203	20.73%	2.260%
33	16.275	2222	2225	2228	rBV5	8457	11954	0.13%	0.014%
34	16.310	2229	2231	2235	rVV2	18882	23648	0.26%	0.028%
35	16.351	2235	2238	2242	rVB6	9850	16818	0.18%	0.020%
36	16.598	2275	2280	2292	rBV	250083	384882	4.17%	0.454%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	16.851	2317	2323	2325	rBV7	14942	23821	0.26%	0.028%
38	16.910	2331	2333	2338	rVB5	9421	12471	0.14%	0.015%
39	17.092	2361	2364	2369	rBV5	17102	27938	0.30%	0.033%
40	17.192	2377	2381	2383	rBV5	7315	11792	0.13%	0.014%
41	17.328	2401	2404	2408	rVB5	13093	14260	0.15%	0.017%
42	17.433	2414	2422	2433	rBV	2189789	3364871	36.43%	3.970%
43	17.539	2434	2440	2466	rVV2	3103262	7691160	83.26%	9.074%
44	18.169	2544	2547	2553	rVV8	17301	31221	0.34%	0.037%
45	18.286	2562	2567	2578	rBV	539891	1133737	12.27%	1.338%
46	19.351	2744	2748	2752	rBV2	61723	82985	0.90%	0.098%
47	19.522	2773	2777	2790	rBV	145560	330482	3.58%	0.390%
48	19.769	2813	2819	2845	rBV2	4087929	9237616	100.00%	10.898%
49	20.233	2895	2898	2902	rBV2	44316	56795	0.61%	0.067%
50	21.169	3055	3057	3060	rBV2	72921	61544	0.67%	0.073%
51	21.227	3060	3067	3081	rBV3	391116	1261832	13.66%	1.489%
52	21.557	3118	3123	3132	rBV	1197683	3061518	33.14%	3.612%
53	22.751	3322	3326	3337	rVB	366715	534335	5.78%	0.630%
54	23.904	3515	3522	3542	rBV2	2465321	6876043	74.44%	8.112%
55	24.086	3547	3553	3573	rVB	747812	2648778	28.67%	3.125%

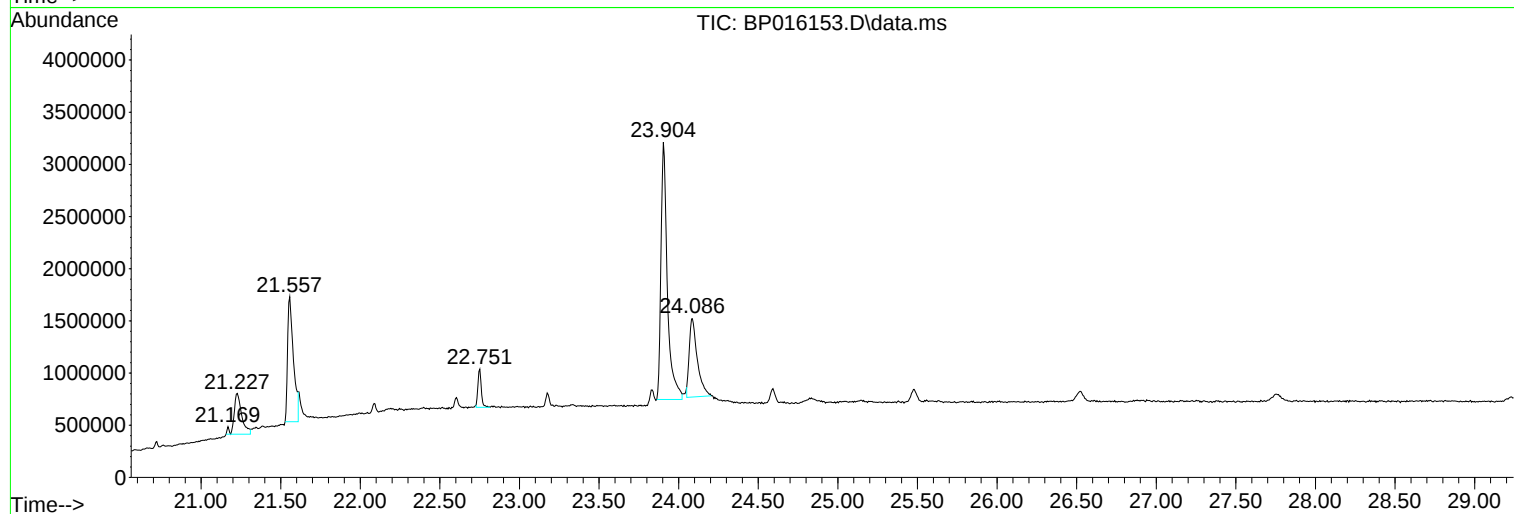
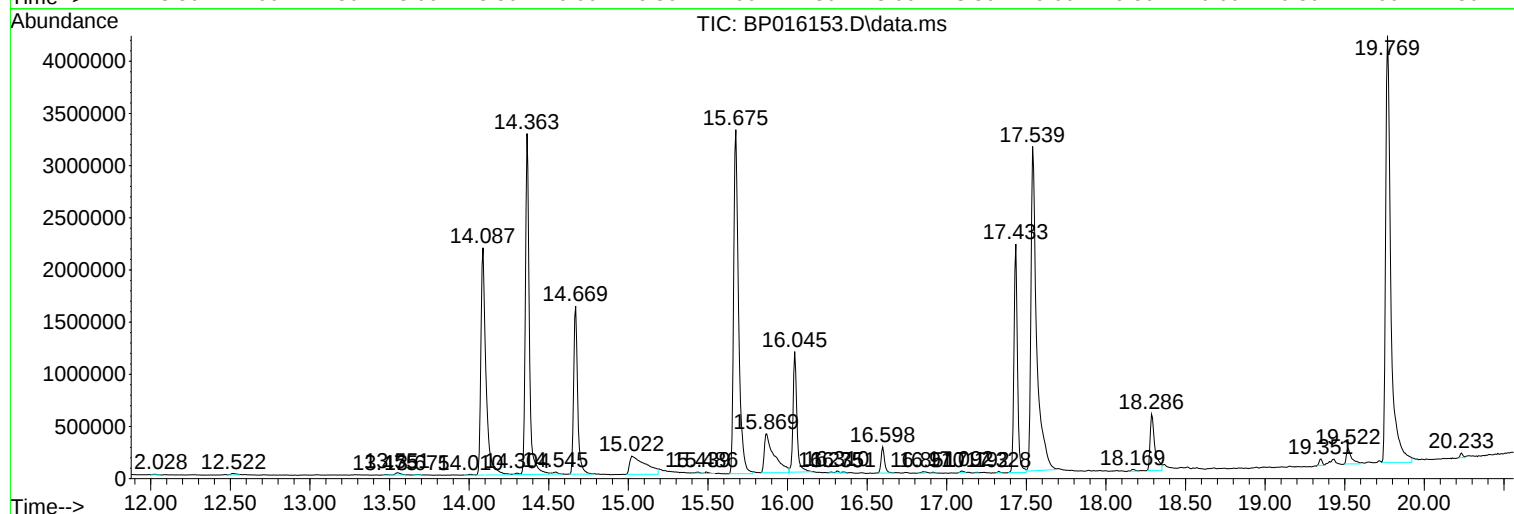
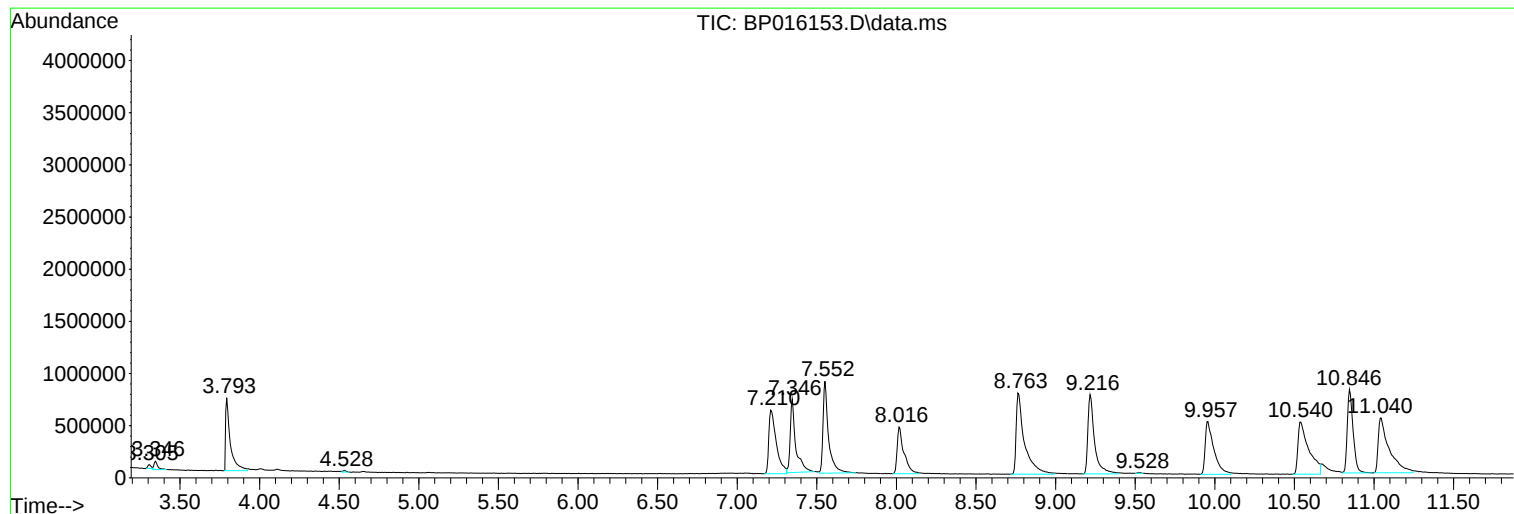
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Quant Title : SVOA CALIBRATION

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



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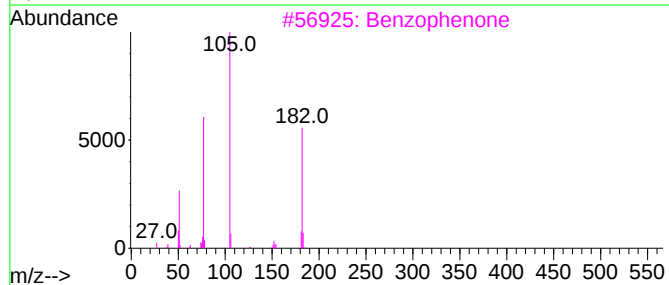
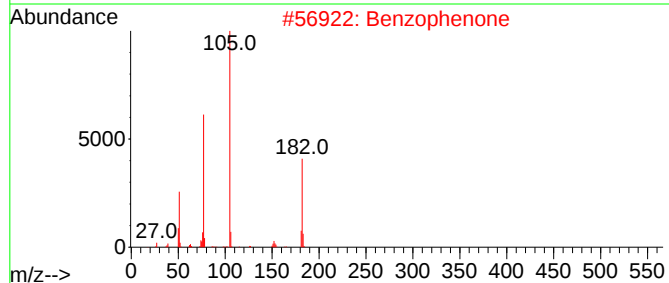
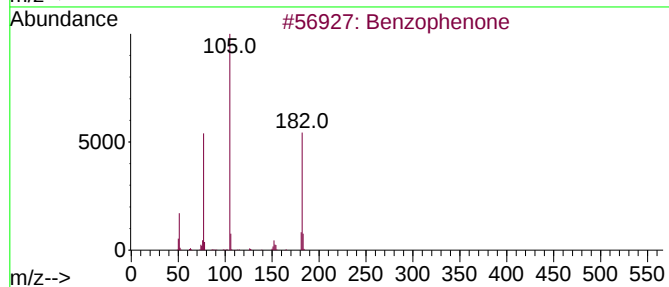
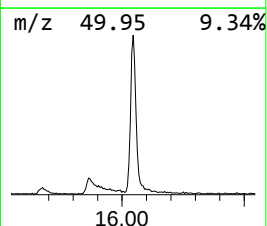
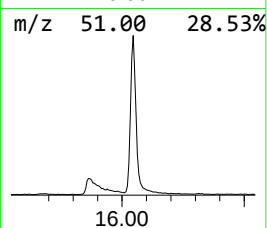
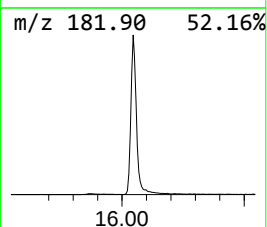
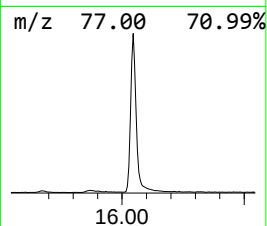
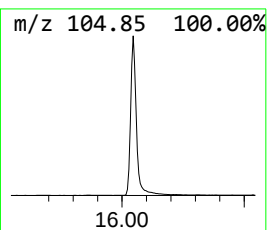
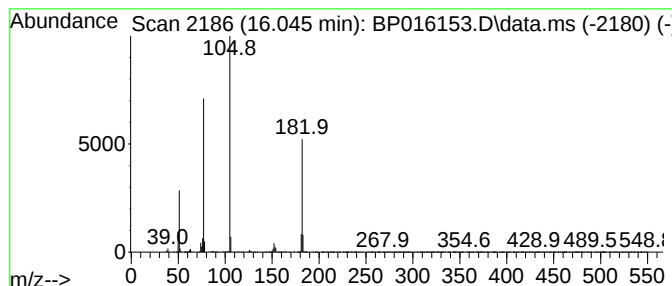
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	13.78 ng/ul	1915200	Acenaphthene-d10	14.669

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	96
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Benzophenone	182	C13H10O	000119-61-9	91



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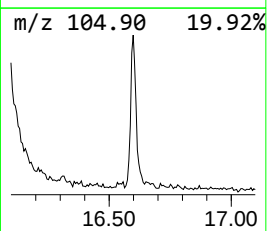
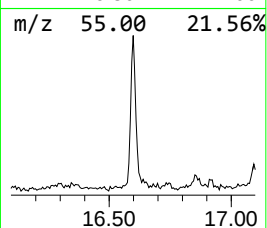
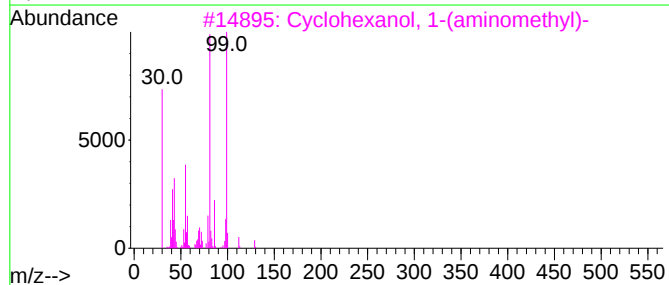
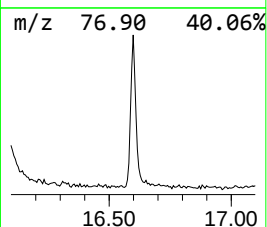
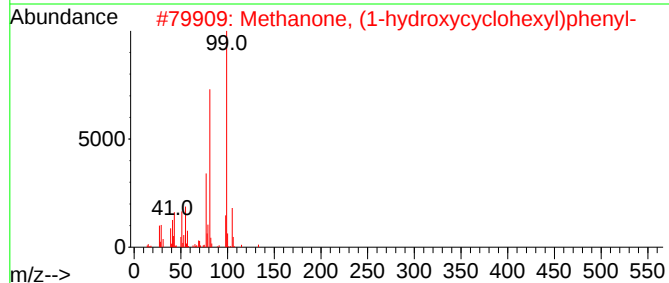
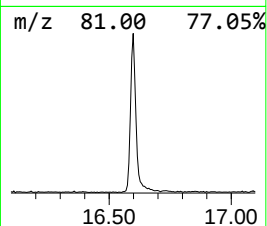
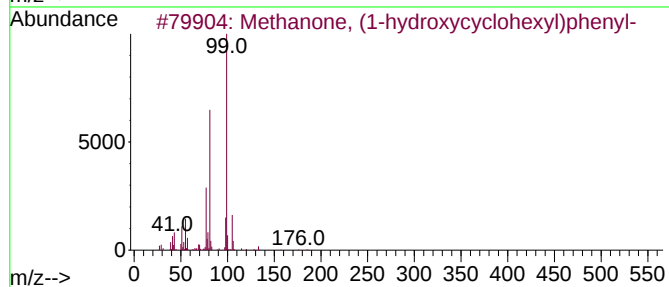
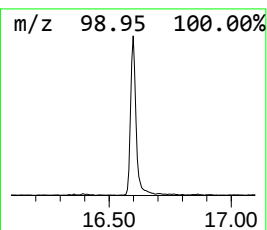
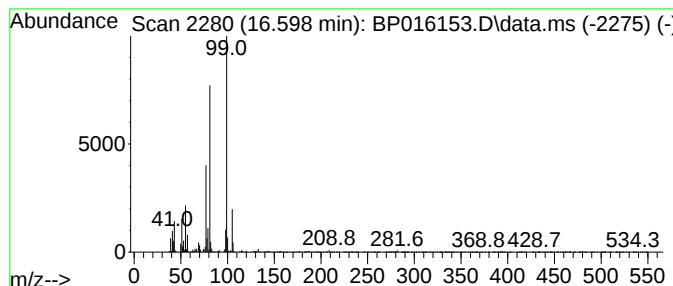
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	2.29 ng/ul	384882	Phenanthrene-d10	17.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	80
3			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	53
4			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	50
5			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	42



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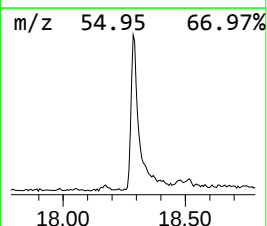
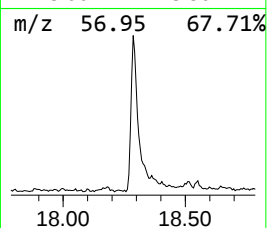
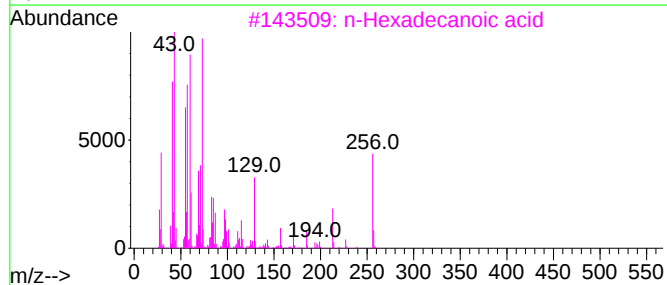
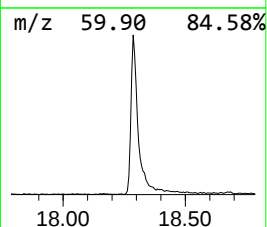
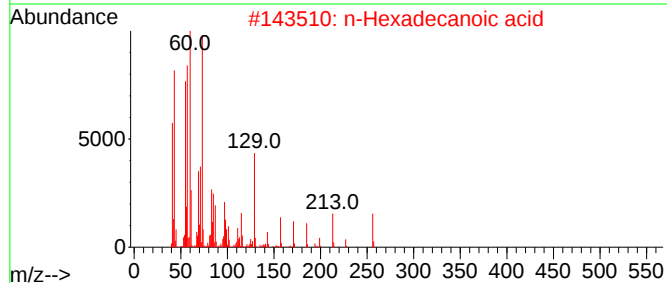
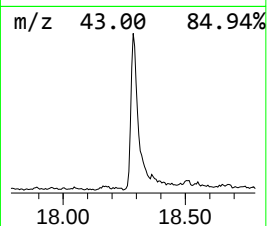
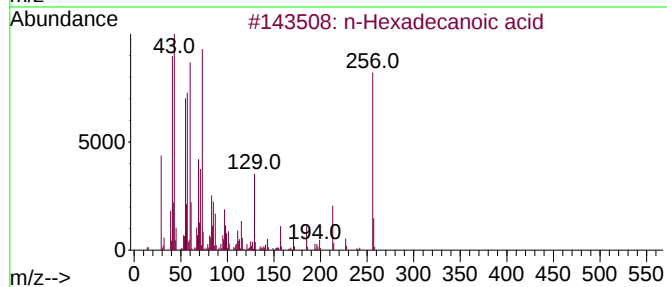
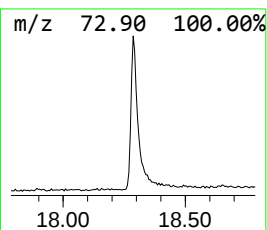
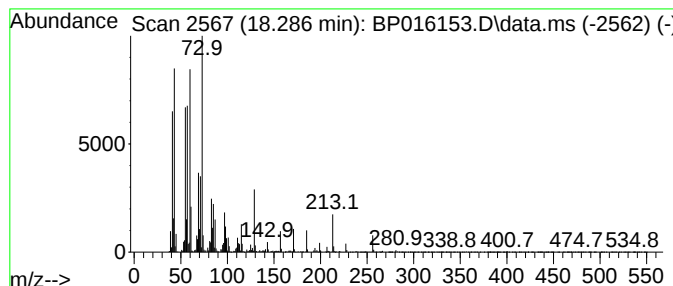
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	6.74 ng/ul	1133740	Phenanthrene-d10	17.433

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			Tridecanoic acid	214	C13H26O2	000638-53-9	94
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	94



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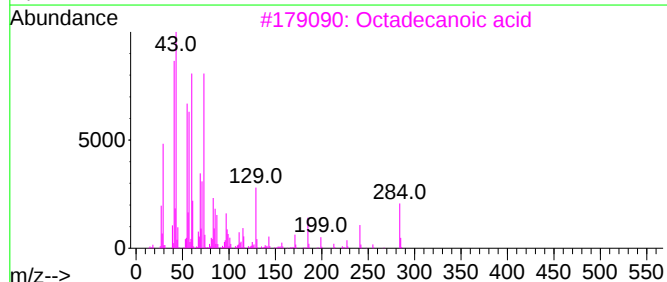
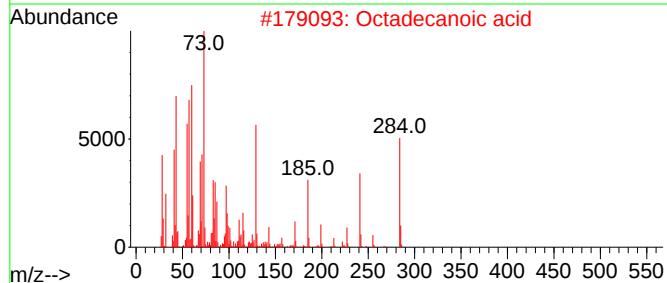
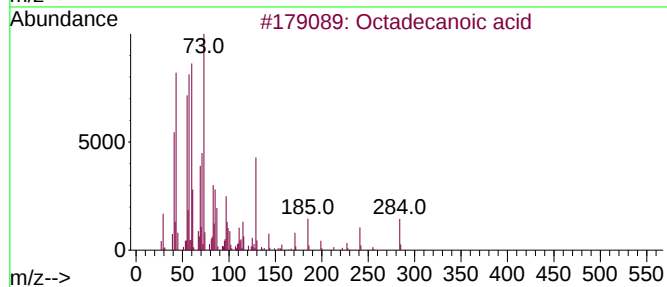
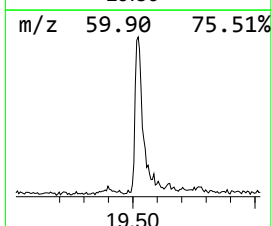
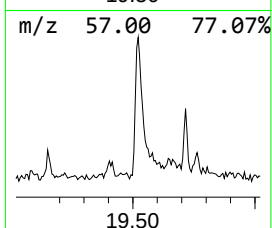
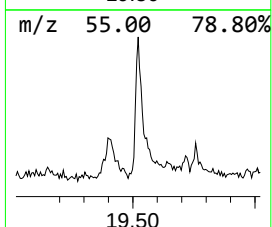
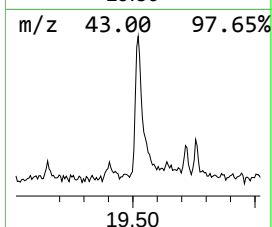
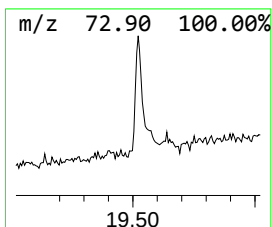
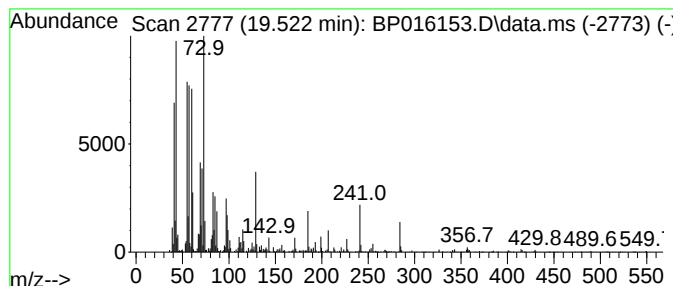
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.522	2.16 ng/ul	330482	Chrysene-d12	21.557

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	96
3			Octadecanoic acid	284	C18H36O2	000057-11-4	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			Heneicosanoic acid	326	C21H42O2	002363-71-5	90



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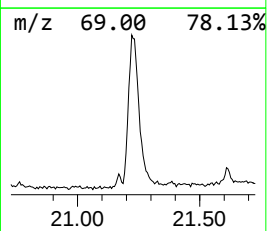
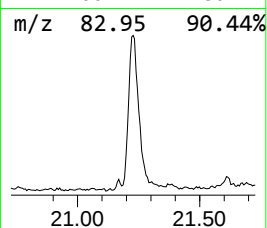
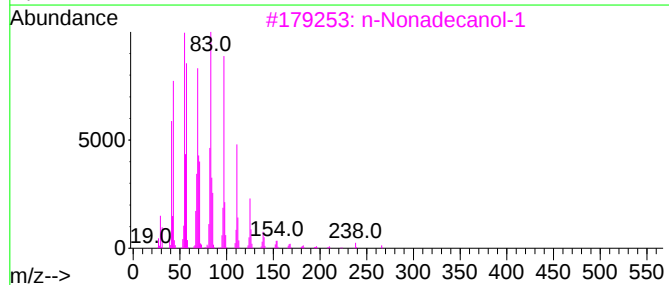
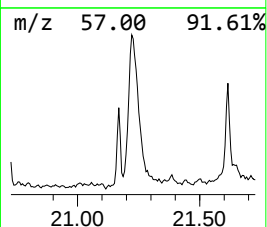
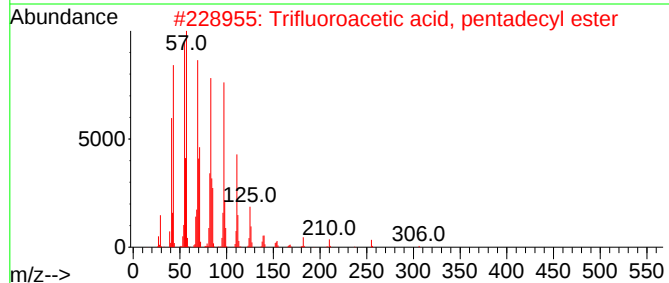
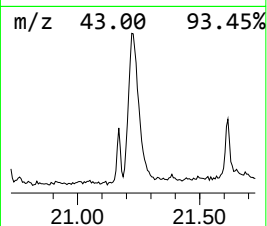
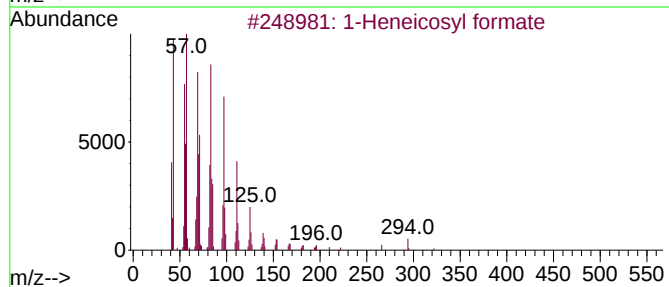
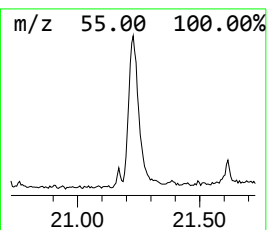
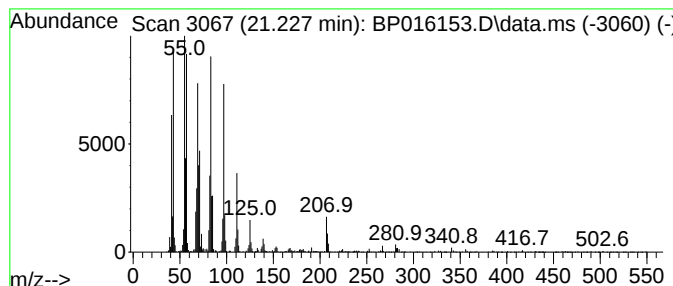
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	8.24 ng/ul	1261830	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016153.D
Acq On : 10 Jul 2023 11:52
Operator : MA/JU
Sample : 03356-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW37

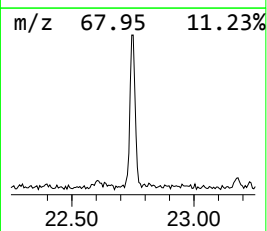
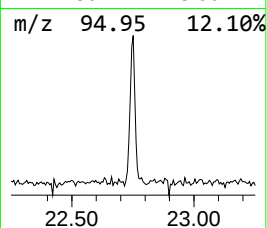
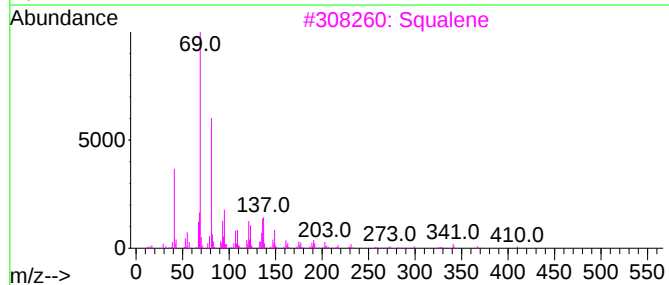
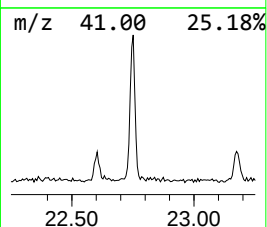
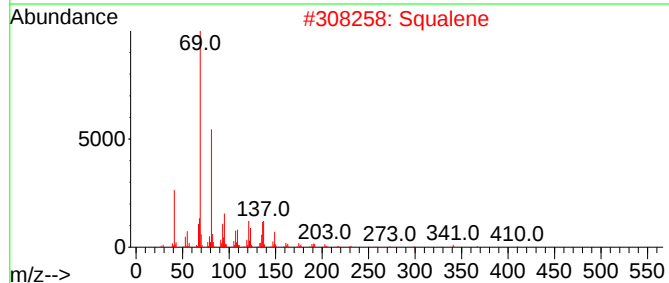
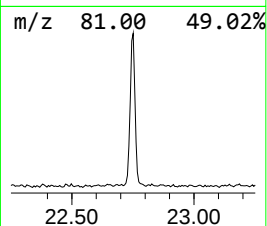
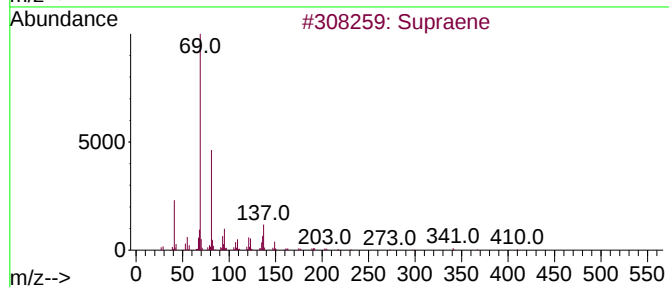
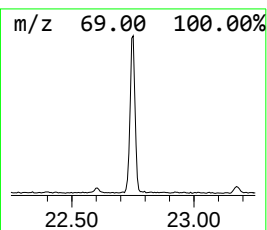
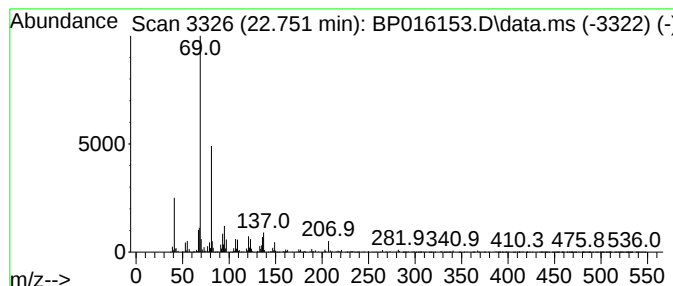
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.751	3.49 ng/ul	534335	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	98
2			Squalene	410	C30H50	000111-02-4	91
3			Squalene	410	C30H50	000111-02-4	68
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016153.D
Acq On : 10 Jul 2023 11:52
Operator : MA/JU
Sample : 03356-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW37

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	16.045	13.8	ng/ul	1915200	3	14.669	2778770	20.0
Methanone, (1-h...	16.598	2.3	ng/ul	384882	4	17.433	3364870	20.0
n-Hexadecanoic ...	18.286	6.7	ng/ul	1133740	4	17.433	3364870	20.0
Octadecanoic acid	19.522	2.2	ng/ul	330482	5	21.557	3061520	20.0
1-Heneicosyl fo...	21.227	8.2	ng/ul	1261830	5	21.557	3061520	20.0
Supraene	22.751	3.5	ng/ul	534335	5	21.557	3061520	20.0