

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
 Data File : BP018718.D
 Acq On : 08 Dec 2023 18:20
 Operator : MA/JU
 Sample : 04929-08
 Misc :
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AQ6

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-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	26	30	36	rVB	57583	70868	1.10%	0.104%
2	3.558	78	80	84	rVB2	19906	19998	0.31%	0.029%
3	3.681	97	101	120	rBV	671330	1006894	15.57%	1.483%
4	3.958	133	148	155	rBV	283244	817620	12.64%	1.204%
5	5.152	345	351	363	rVB	276904	421920	6.52%	0.622%
6	5.287	371	374	377	rVB	16430	17496	0.27%	0.026%
7	5.340	379	383	388	rVB3	27730	37323	0.58%	0.055%
8	6.675	606	610	614	rBV3	5377	11669	0.18%	0.017%
9	6.864	634	642	652	rBV	117759	231170	3.57%	0.341%
10	7.011	661	667	677	rVB	833146	1326892	20.51%	1.955%
11	7.181	690	696	707	rVB	685643	1046694	16.18%	1.542%
12	7.375	722	729	738	rVB	819629	1334206	20.63%	1.965%
13	7.458	738	743	748	rBV2	11794	23594	0.36%	0.035%
14	7.534	751	756	757	rBV2	10892	14133	0.22%	0.021%
15	7.605	767	768	770	rVB	13881	9269	0.14%	0.014%
16	7.728	783	789	797	rBV	255347	424533	6.56%	0.625%
17	7.846	802	809	811	rVV	662809	1034415	15.99%	1.524%
18	7.881	811	815	824	rVB	834610	1326164	20.50%	1.954%
19	8.193	862	868	876	rBV	772538	1218028	18.83%	1.794%
20	8.552	922	929	938	rBV	1039827	1642171	25.39%	2.419%
21	9.005	999	1006	1014	rBV	746610	1190621	18.41%	1.754%
22	9.169	1030	1034	1038	rVB4	10754	16053	0.25%	0.024%
23	9.240	1043	1046	1051	rVB4	8121	13430	0.21%	0.020%
24	9.416	1073	1076	1080	rBV4	5953	8594	0.13%	0.013%
25	9.722	1121	1128	1136	rBV	554405	908419	14.04%	1.338%
26	9.781	1136	1138	1145	rVB4	16024	25484	0.39%	0.038%
27	10.075	1186	1188	1192	rBV4	4870	6999	0.11%	0.010%
28	10.257	1212	1219	1230	rBV	985011	1646175	25.45%	2.425%
29	10.505	1254	1261	1267	rBV	407707	674759	10.43%	0.994%
30	10.640	1277	1284	1291	rVB	901844	1473257	22.78%	2.170%
31	10.781	1299	1308	1319	rBV	920130	1637431	25.31%	2.412%
32	11.022	1343	1349	1356	rVB2	48210	85717	1.33%	0.126%
33	11.440	1417	1420	1423	rBV5	4830	6584	0.10%	0.010%
34	11.763	1472	1475	1478	rBV2	5500	10159	0.16%	0.015%
35	11.822	1478	1485	1486	rVV3	10410	21231	0.33%	0.031%
36	11.910	1497	1500	1503	rBV2	5549	8326	0.13%	0.012%

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37	11.993	1513	1514	1518	rVB	16417	13103	0.20%	0.019%
38	12.069	1518	1527	1529	rVB3	4484	8352	0.13%	0.012%
39	12.228	1547	1554	1559	rBV3	18008	33914	0.52%	0.050%
40	12.440	1584	1590	1596	rBV3	11367	21846	0.34%	0.032%

41	12.634	1618	1623	1625	rBV3	9239	16228	0.25%	0.024%
42	12.663	1625	1628	1633	rVB2	29467	45938	0.71%	0.068%
43	13.275	1726	1732	1737	rBV	62496	104303	1.61%	0.154%
44	13.375	1744	1749	1755	rBV2	27827	49355	0.76%	0.073%
45	13.446	1758	1761	1766	rVB7	10083	13863	0.21%	0.020%

46	13.493	1766	1769	1773	rBV4	5143	8588	0.13%	0.013%
47	13.887	1830	1836	1843	rBV	1717065	2357497	36.45%	3.473%
48	14.163	1877	1883	1893	rBV	1968669	2958215	45.73%	4.358%
49	14.475	1929	1936	1946	rVB	1313669	1981507	30.63%	2.919%
50	14.675	1963	1970	1983	rBV	753971	1200145	18.55%	1.768%

51	14.893	2004	2007	2012	rVB7	13186	18501	0.29%	0.027%
52	15.463	2098	2104	2113	rBV	2782066	3944137	60.98%	5.810%
53	15.581	2118	2124	2137	rVV	575564	808841	12.50%	1.191%
54	15.704	2142	2145	2152	rVB2	16373	23718	0.37%	0.035%
55	16.251	2235	2238	2242	rBV5	6455	7330	0.11%	0.011%

56	16.463	2272	2274	2280	rVB2	9006	12112	0.19%	0.018%
57	17.222	2397	2403	2409	rBV	1792929	2574333	39.80%	3.792%
58	17.322	2413	2420	2430	rVV	3255728	4584062	70.87%	6.753%
59	17.416	2433	2436	2442	rVB3	24434	36725	0.57%	0.054%
60	17.863	2508	2512	2515	rBV3	26850	38585	0.60%	0.057%

61	18.110	2550	2554	2565	rBV	289048	439189	6.79%	0.647%
62	18.292	2581	2585	2595	rVB9	40669	81509	1.26%	0.120%
63	18.498	2615	2620	2627	rBV	472466	612987	9.48%	0.903%
64	18.557	2627	2630	2637	rVB7	27723	44343	0.69%	0.065%
65	18.798	2667	2671	2677	rVB3	104524	127532	1.97%	0.188%

66	19.016	2703	2708	2717	rVB	380757	491560	7.60%	0.724%
67	19.133	2724	2728	2735	rBV3	52085	80488	1.24%	0.119%
68	19.204	2736	2740	2743	rBV	63642	85728	1.33%	0.126%
69	19.345	2760	2764	2775	rBV2	144738	186961	2.89%	0.275%
70	19.557	2794	2800	2807	rBV	4543553	6396261	98.89%	9.422%

71	19.704	2821	2825	2828	rBV	132647	157569	2.44%	0.232%
72	19.745	2829	2832	2835	rBV4	49455	64462	1.00%	0.095%
73	20.086	2887	2890	2894	rVB4	95917	112755	1.74%	0.166%
74	20.245	2912	2917	2931	rBV3	389620	1056487	16.33%	1.556%
75	20.451	2948	2952	2960	rBV2	649840	936451	14.48%	1.379%

76	20.528	2963	2965	2967	rVV2	86154	100227	1.55%	0.148%
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Title : SVOA CALIBRATION

77	20.569	2967	2972	2987	rVB4	531179	1185713	18.33%	1.747%
78	20.763	3000	3005	3016	rVB	1007296	1338215	20.69%	1.971%
79	20.857	3018	3021	3027	rVB5	124376	166034	2.57%	0.245%
80	21.033	3047	3051	3060	rVB4	242100	439503	6.79%	0.647%
81	21.310	3093	3098	3103	rBV	2561262	3220904	49.79%	4.745%
82	23.521	3467	3474	3481	rBV2	3323288	6468342	100.00%	9.528%
83	23.674	3494	3500	3511	rVB	1779830	3461846	53.52%	5.100%

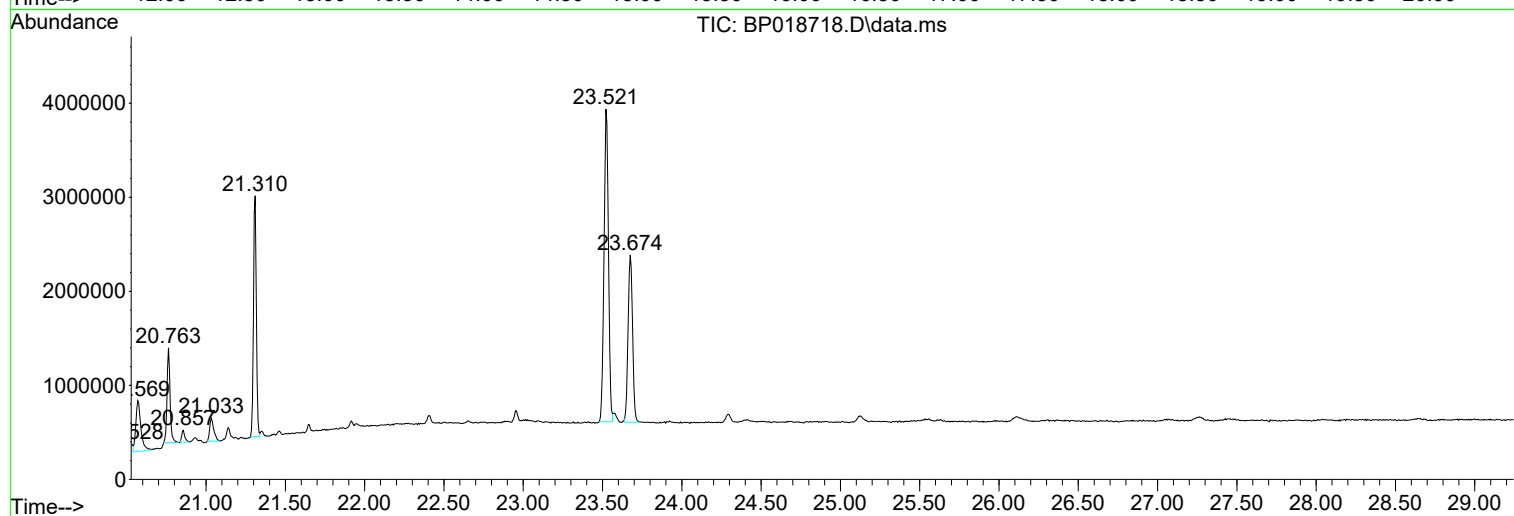
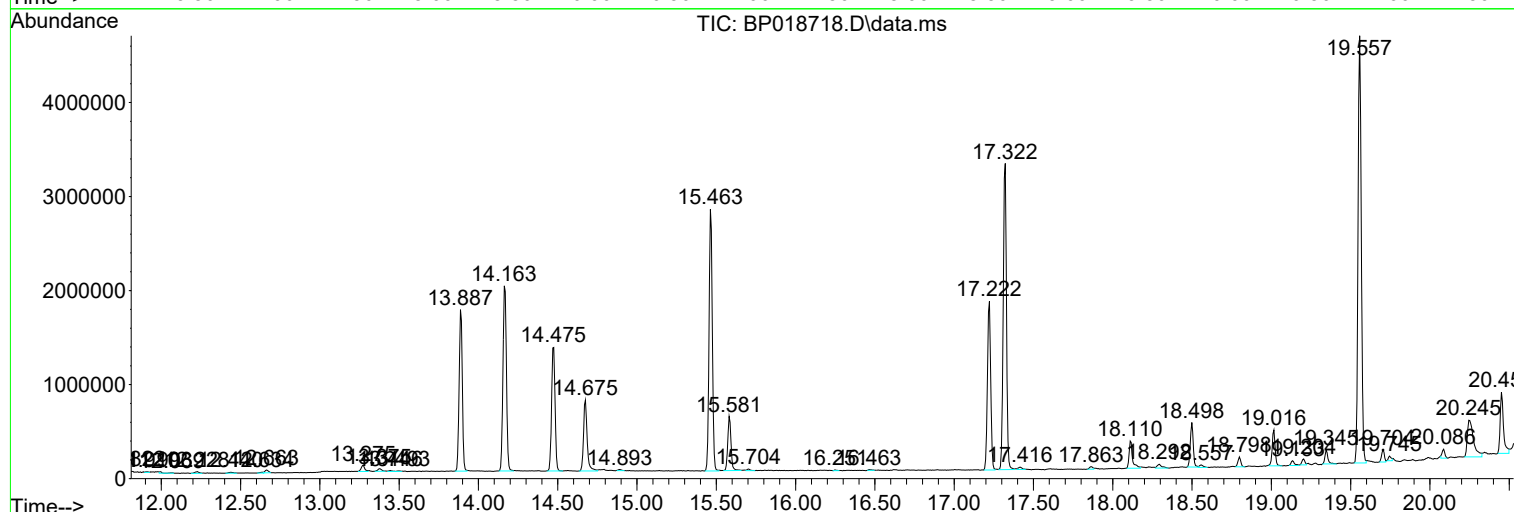
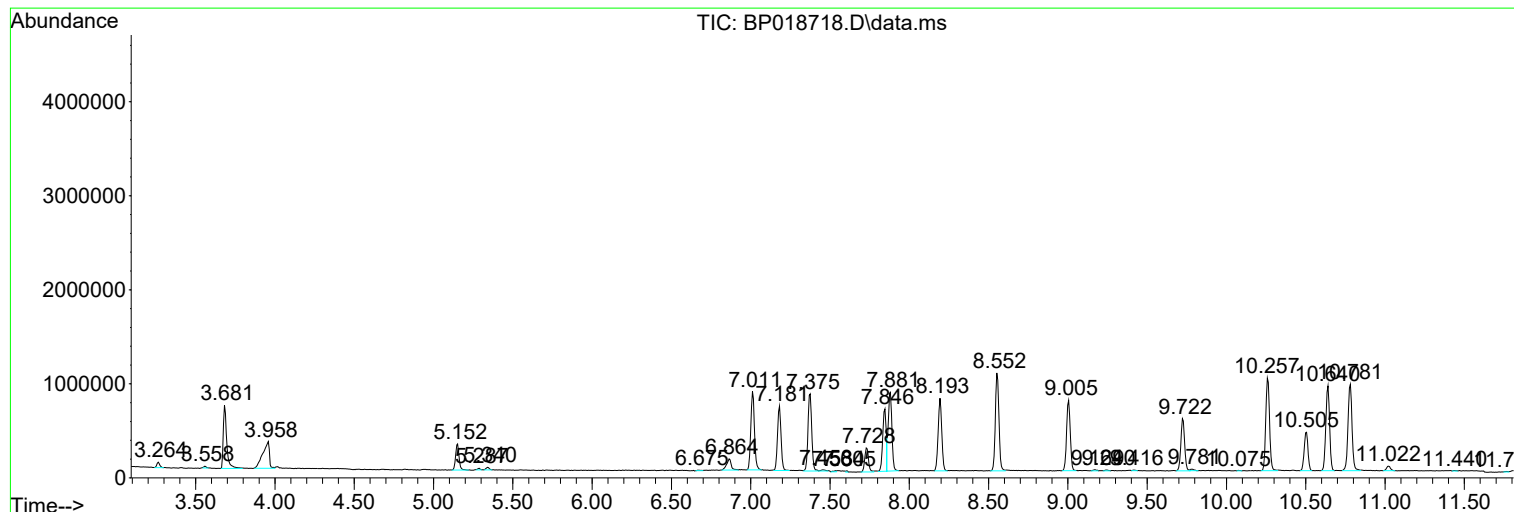
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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



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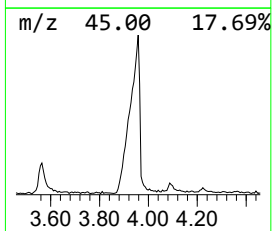
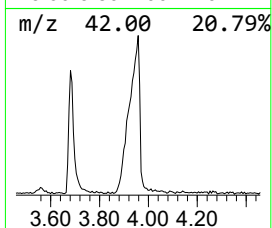
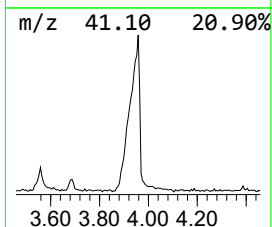
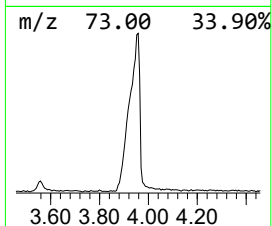
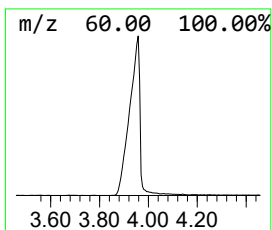
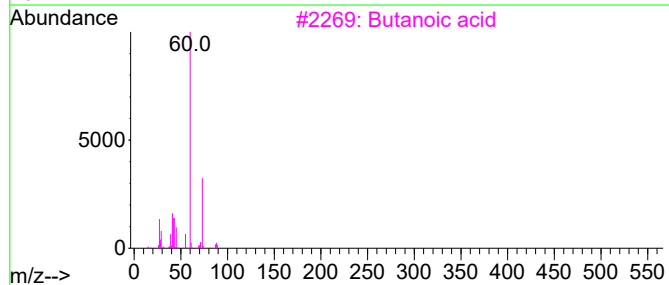
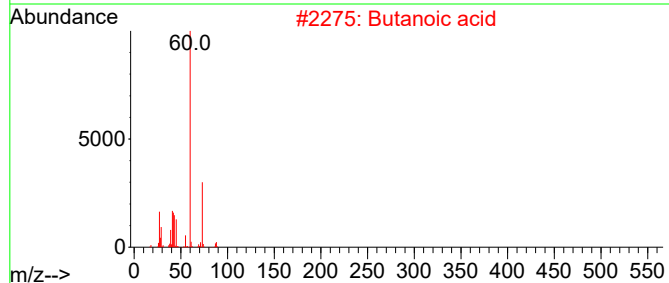
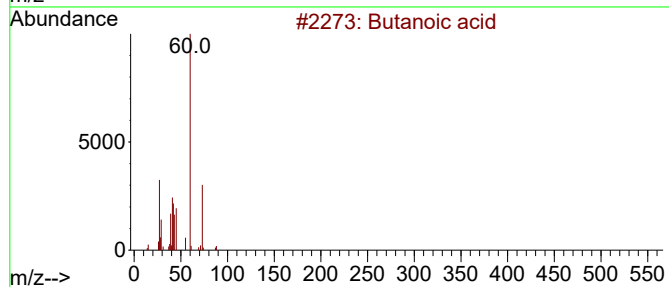
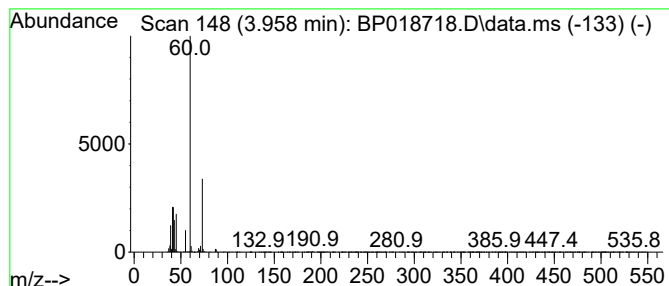
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.958	15.81 ng/ul	817620	1,4-Dichlorobenzene-d4	7.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Butanoic acid	88	C4H8O2	000107-92-6	86
3			Butanoic acid	88	C4H8O2	000107-92-6	72
4			Pentanoic acid	102	C5H10O2	000109-52-4	72
5			Butanoic acid	88	C4H8O2	000107-92-6	72



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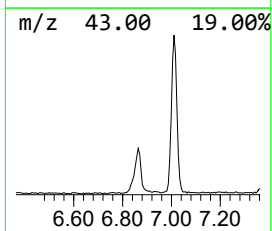
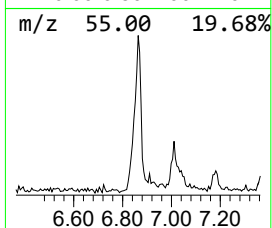
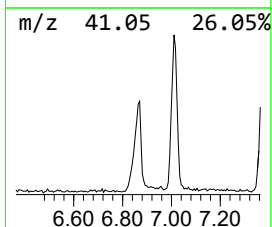
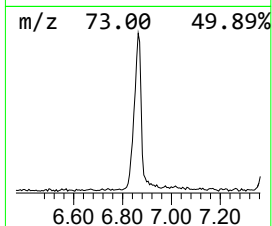
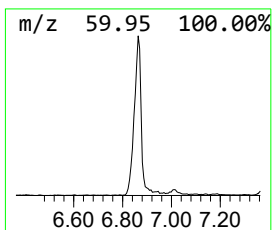
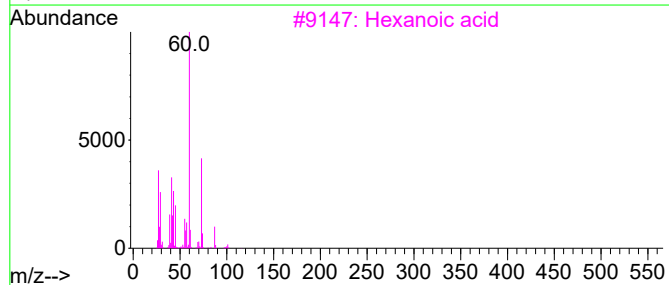
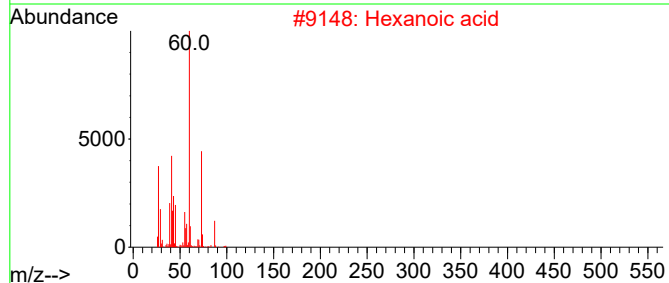
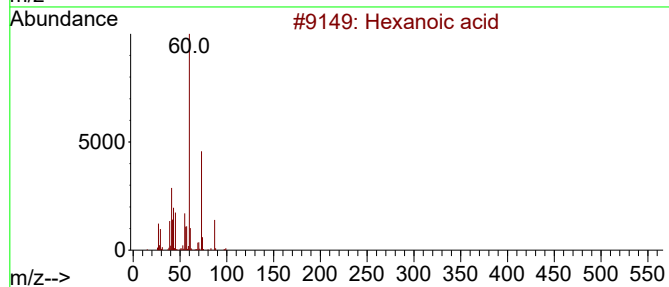
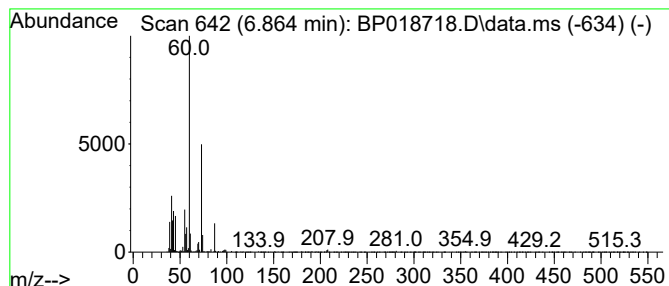
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Hexanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.864	4.47 ng/ul	231170	1,4-Dichlorobenzene-d4	7.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	83
3			Hexanoic acid	116	C6H12O2	000142-62-1	83
4			Octanoic acid	144	C8H16O2	000124-07-2	74
5			Pentanoic acid	102	C5H10O2	000109-52-4	72



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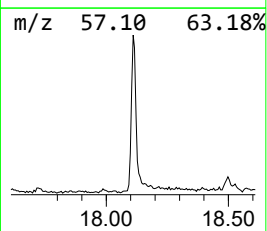
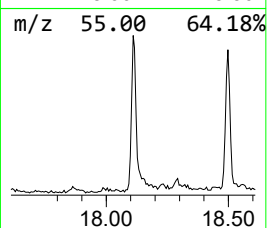
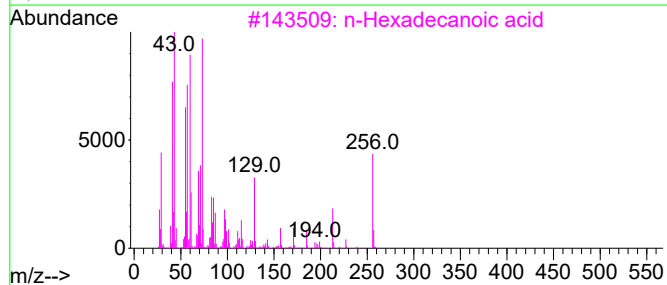
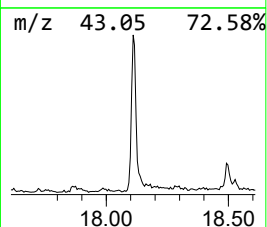
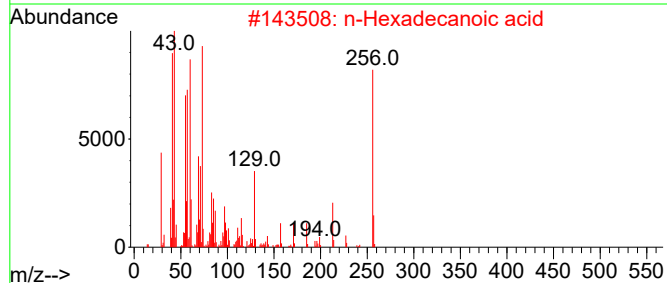
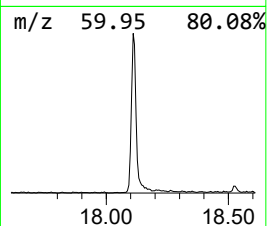
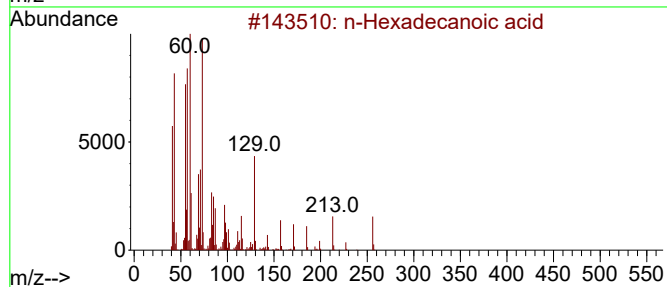
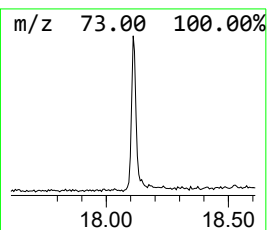
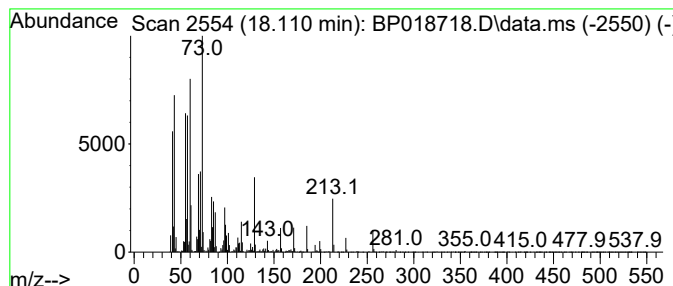
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.110	3.41 ng/ul	439189	Phenanthrene-d10	17.222

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			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



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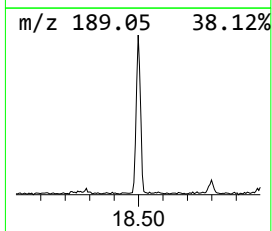
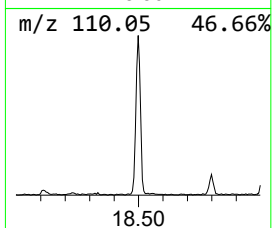
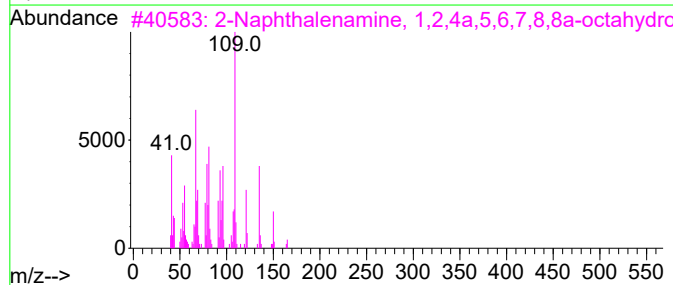
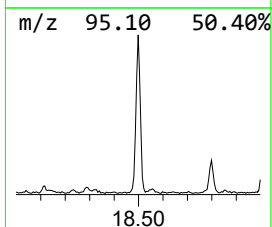
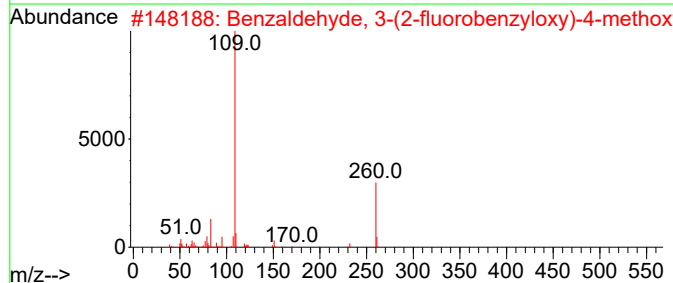
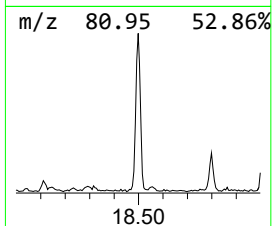
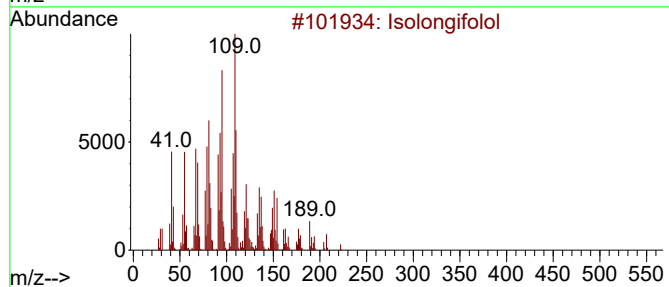
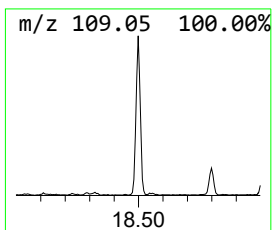
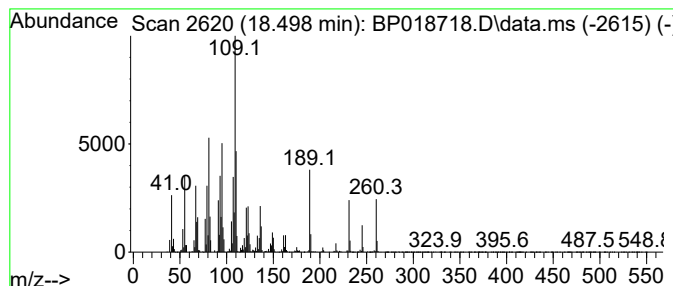
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.498	4.76 ng/ul	612987	Phenanthrene-d10	17.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isolongifolol	222	C15H26O	001139-17-9	27
2			Benzaldehyde, 3-(2-fluorobenzilo...	260	C15H13FO3	1000276-29-6	22
3			2-Naphthalenamine, 1,2,4a,5,6,7,...	165	C11H19N	056053-03-3	22
4			1H-Pyrazole-5-carboxamide, N-(3-...	231	C12H13N3O2	1000319-53-5	22
5			4-Pyrimidinamine, 6-methyl-	109	C5H7N3	003435-28-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ6

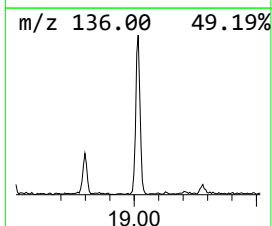
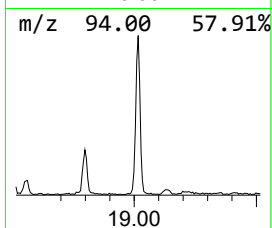
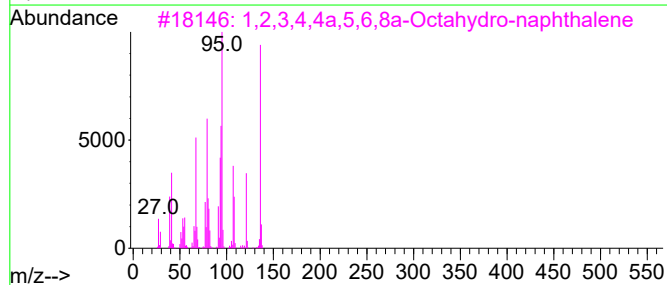
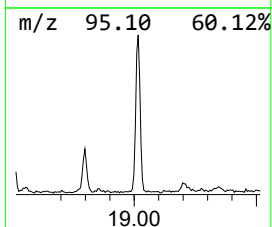
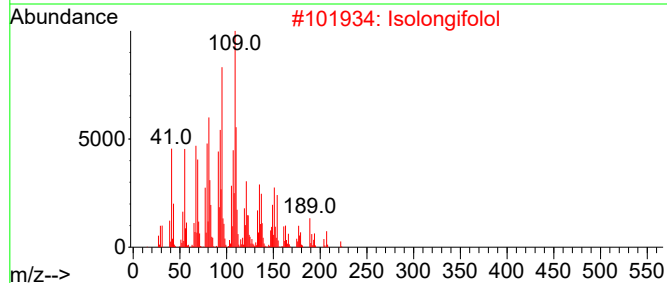
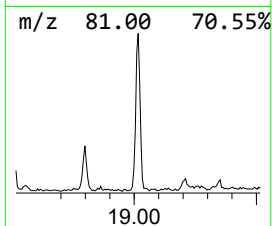
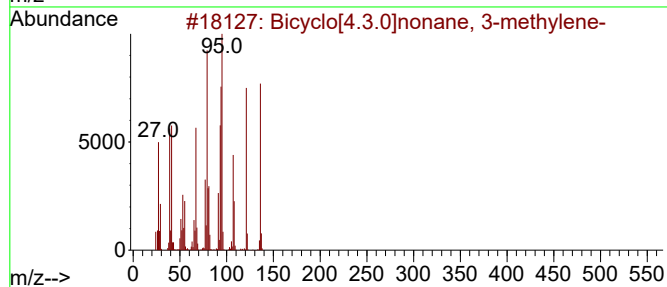
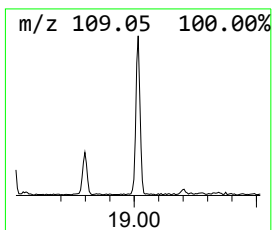
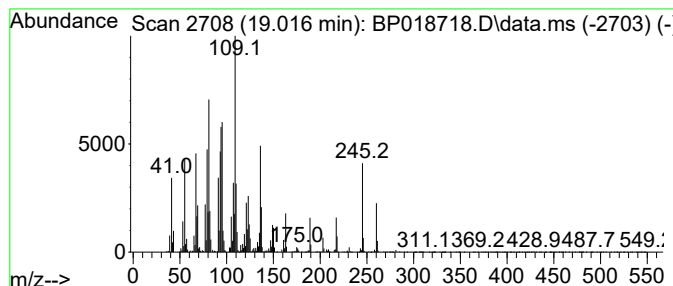
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-02 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.016	3.82 ng/ul	491560	Phenanthrene-d10	17.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.3.0]nonane, 3-methylene-	136	C10H16	1000152-00-6	42
2			Isolongifolol	222	C15H26O	001139-17-9	35
3			1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	30
4			1(3H)-Isobenzofuranone, 3a,4,5,7...	182	C10H14O3	054346-06-4	27
5			Bornyl acetate	196	C12H20O2	000076-49-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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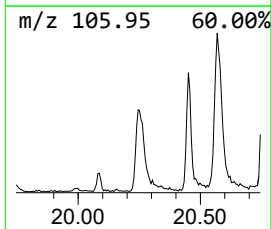
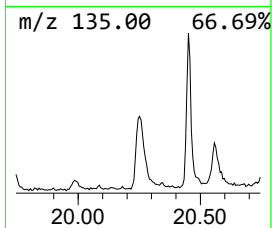
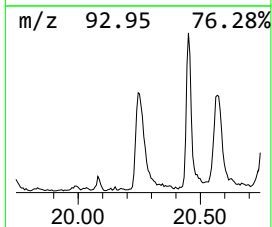
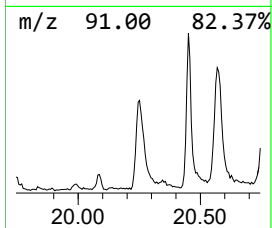
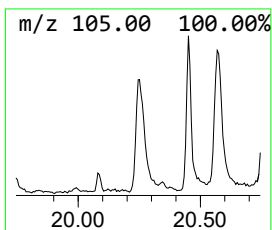
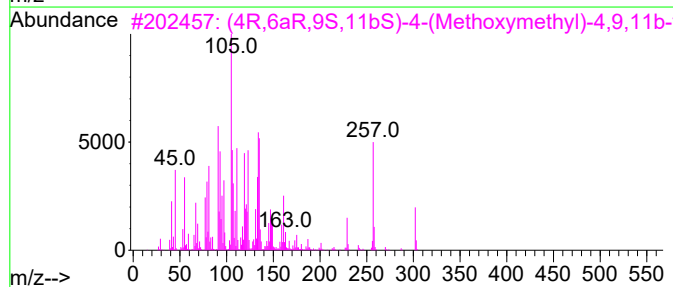
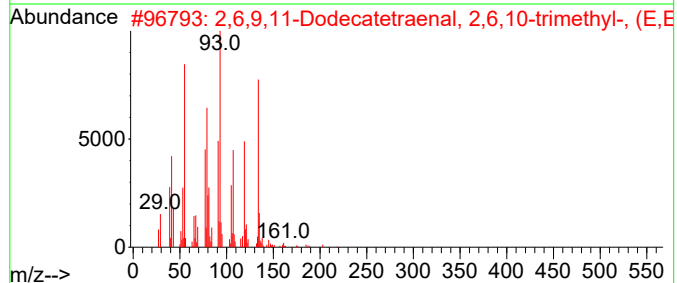
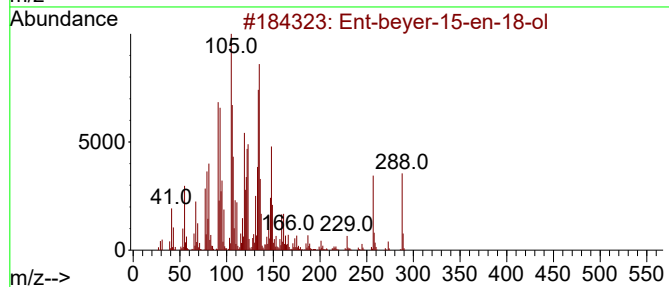
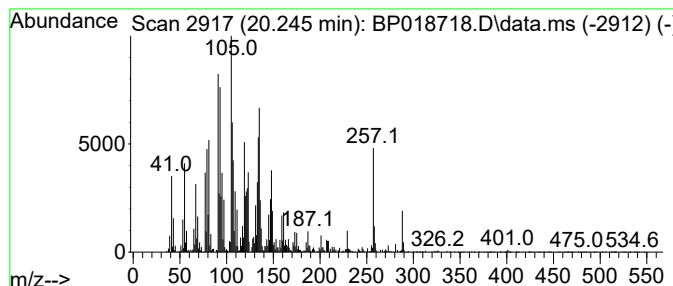
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Ent-beyer-15-en-18-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.245	6.56 ng/ul	1056490	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ent-beyer-15-en-18-ol	288	C20H32O	020107-90-8	50
2			2,6,9,11-Dodecatetraenal, 2,6,10...	218	C15H22O	017909-77-2	43
3			(4R,6aR,9S,11bS)-4-(Methoxymethy...	302	C21H34O	1000495-78-0	38
4			10,13-Octadecadiynoic acid, meth...	290	C19H30O2	018202-24-9	38
5			N-Tert-butylaniline	149	C10H15N	1000423-71-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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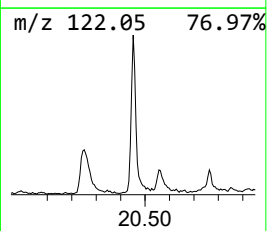
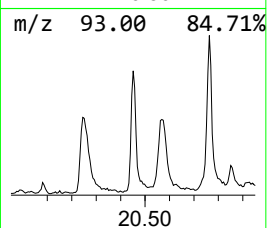
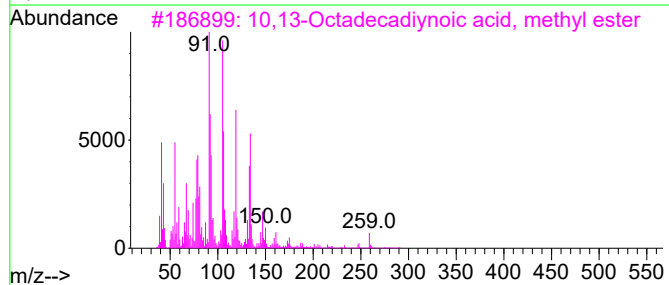
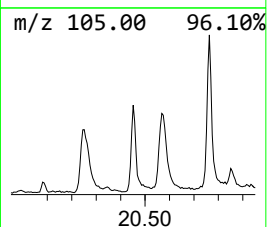
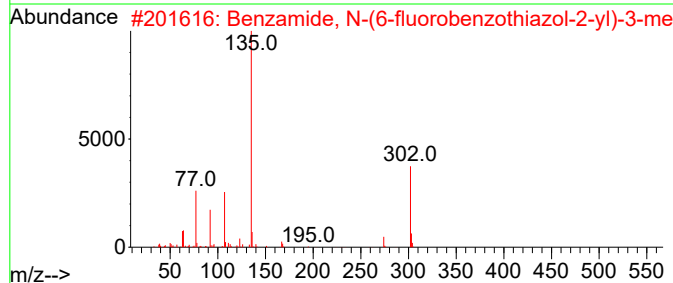
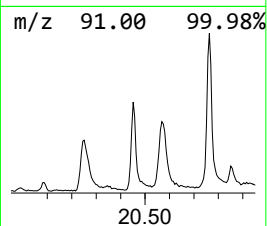
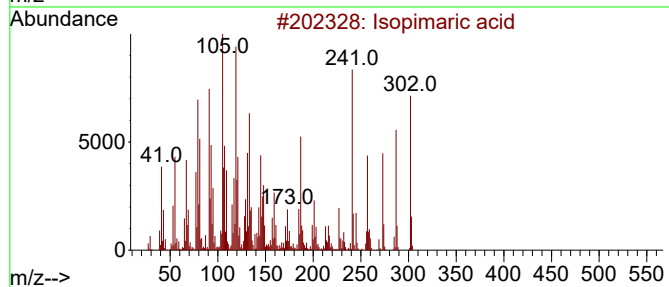
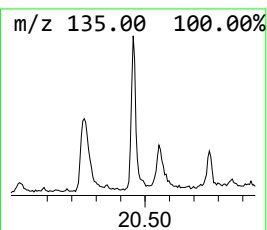
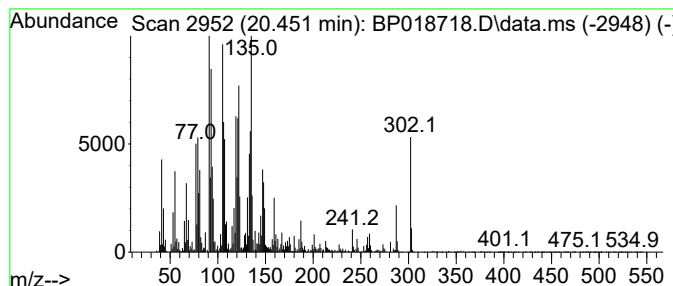
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 Isopimaric acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.451	5.81 ng/ul	936451	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopimaric acid	302	C20H30O2	005835-26-7	58
2			Benzamide, N-(6-fluorobenzothiaz...	302	C15H11FN2O2S	1000304-71-2	38
3			10,13-Octadecadiynoic acid, meth...	290	C19H30O2	018202-24-9	30
4			Cyclopropane, 1-bromo-2,2,3,3-te...	214	C10H15Br	138777-60-3	30
5			1-Phenanthrenecarboxylic acid, 1...	302	C20H30O2	000471-77-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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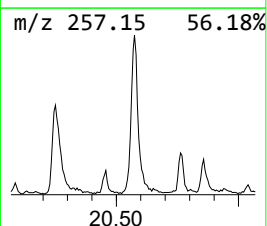
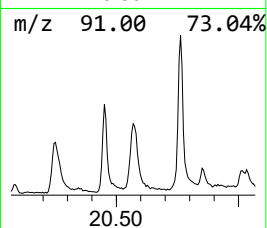
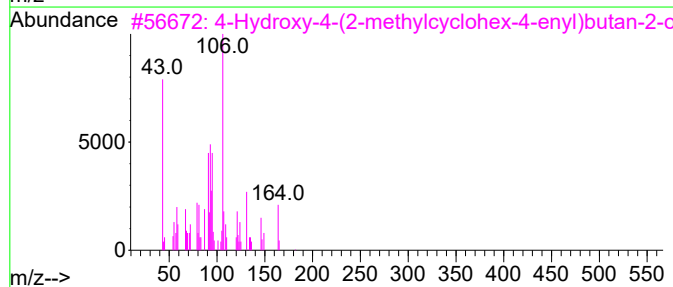
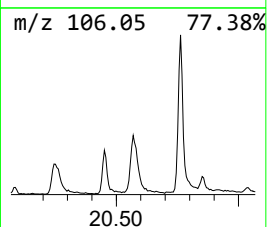
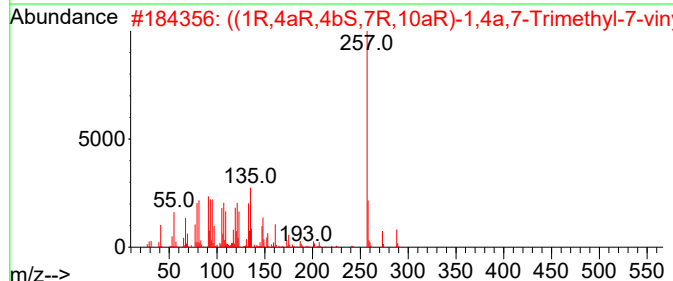
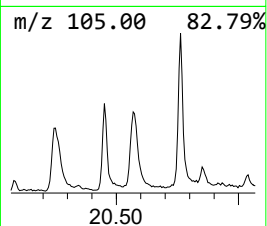
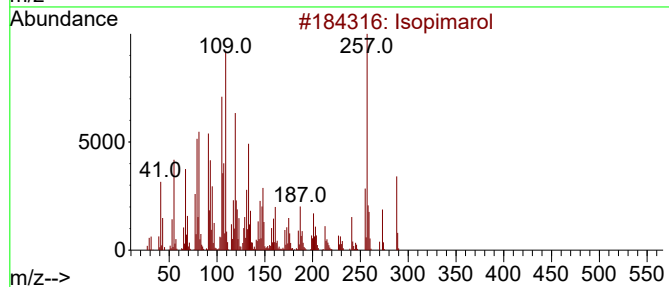
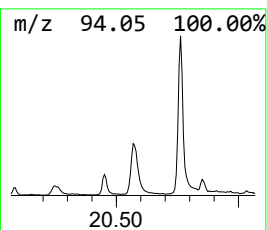
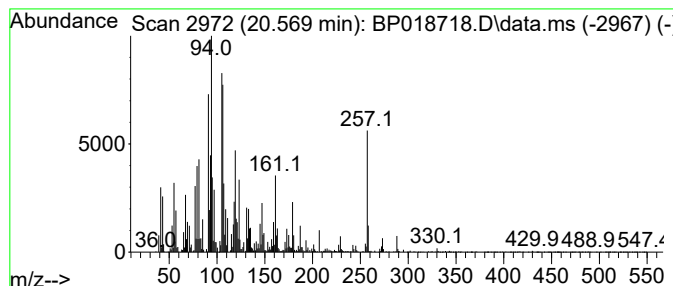
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.569	7.36 ng/ul	1185710	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopimarol	288	C20H32O	001686-64-2	27
2			((1R,4aR,4bS,7R,10aR)-1,4a,7-Tri...	288	C20H32O	024563-84-6	25
3			4-Hydroxy-4-(2-methylcyclohex-4-...	182	C11H18O2	002316-77-0	25
4			cis-2-(Methyl-phenyl)amino-2-thi...	257	C11H16N02PS	1000145-42-9	25
5			(Z)-epi-.beta.-Santalol	220	C15H24O	079081-90-6	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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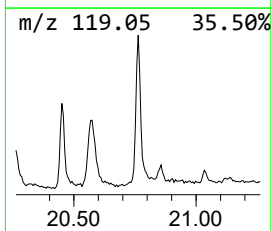
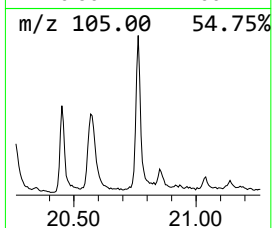
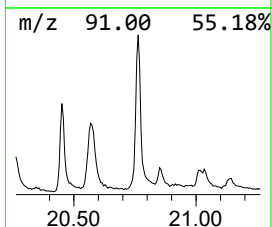
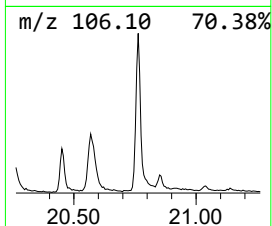
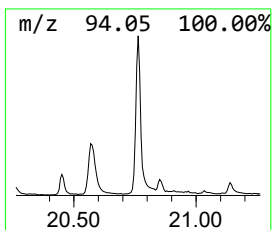
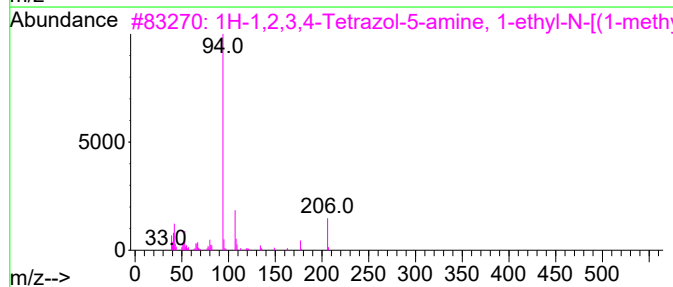
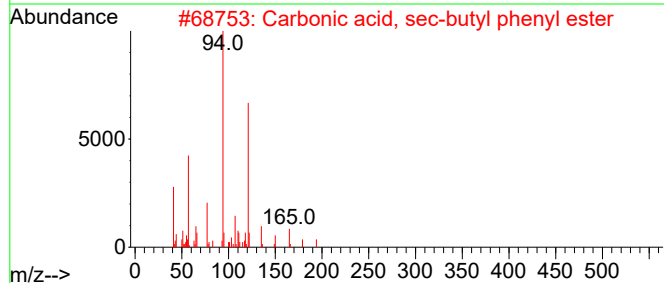
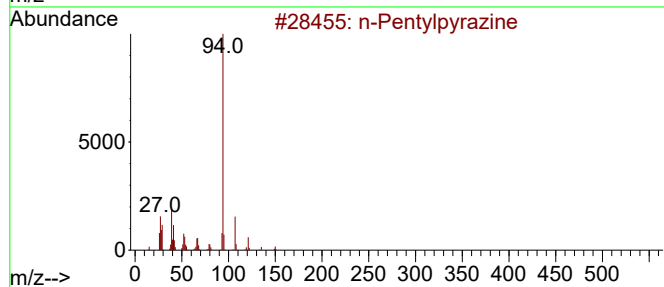
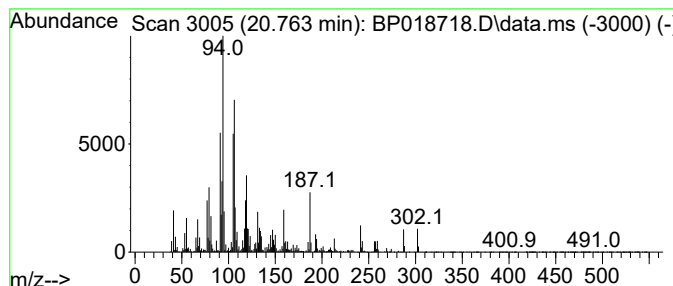
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 unknown-04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.763	8.31 ng/ul	1338220	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Pentylpyrazine	150	C9H14N2	006303-75-9	27
2			Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	27
3			1H-1,2,3,4-Tetrazol-5-amine, 1-e...	206	C9H14N6	1000318-74-7	27
4			Santalol, E-cis, epi-.beta.-	220	C15H24O	014490-17-6	27
5			(Z)-epi-.beta.-Santalol	220	C15H24O	079081-90-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ6

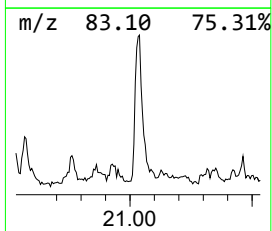
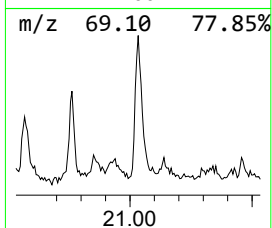
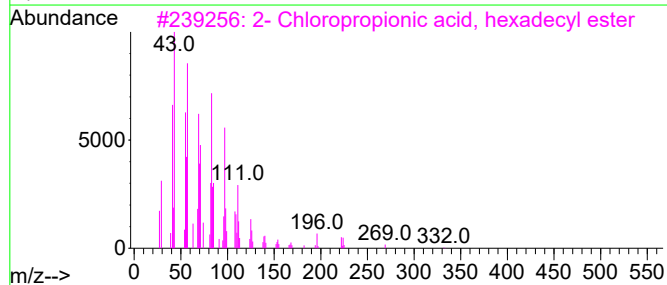
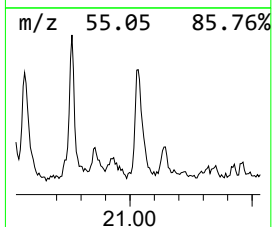
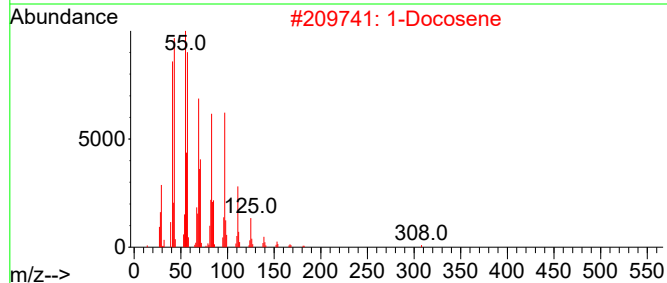
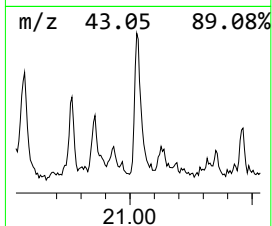
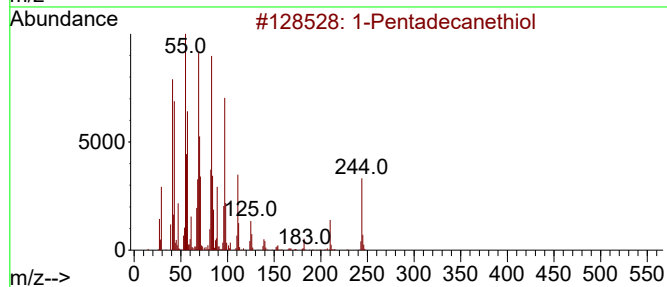
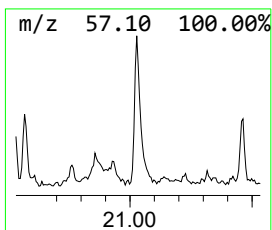
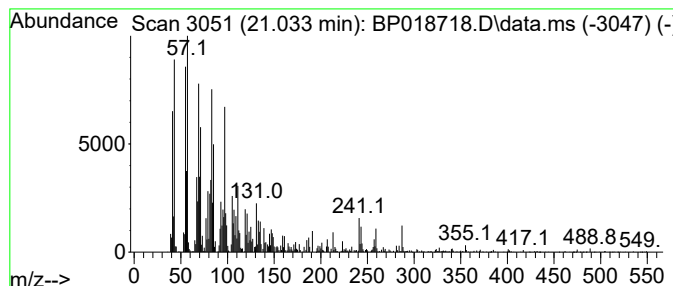
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 14 1-Pentadecanethiol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	2.73 ng/ul	439503	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanethiol	244	C15H32S	025276-70-4	96
2			1-Docosene	308	C22H44	001599-67-3	91
3			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	86
4			Cyclotridecane	182	C13H26	000295-02-3	70
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120723\
Data File : BP018718.D
Acq On : 08 Dec 2023 18:20
Operator : MA/JU
Sample : 04929-08
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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
Butanoic acid	3.958	15.8	ng/ul	817620	1	7.846	1034420	20.0
Hexanoic acid	6.864	4.5	ng/ul	231170	1	7.846	1034420	20.0
n-Hexadecanoic ...	18.110	3.4	ng/ul	439189	4	17.222	2574330	20.0
unknown-01	18.498	4.8	ng/ul	612987	4	17.222	2574330	20.0
unknown-02	19.016	3.8	ng/ul	491560	4	17.222	2574330	20.0
Ent-beyer-15-en...	20.245	6.6	ng/ul	1056490	5	21.310	3220900	20.0
Isopimaric acid	20.451	5.8	ng/ul	936451	5	21.310	3220900	20.0
unknown-03	20.569	7.4	ng/ul	1185710	5	21.310	3220900	20.0
unknown-04	20.763	8.3	ng/ul	1338220	5	21.310	3220900	20.0
1-Pentadecanethiol	21.033	2.7	ng/ul	439503	5	21.310	3220900	20.0