

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
 Data File : BP015778.D
 Acq On : 28 Jun 2023 14:24
 Operator : MA/JU
 Sample : 03142-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFS0

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: BP015778.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	31	33	39	rVB	20818	25447	0.26%	0.070%
2	3.834	106	110	114	rBV2	12189	17301	0.18%	0.047%
3	3.934	123	127	134	rVB	56274	73007	0.75%	0.200%
4	4.051	143	147	155	rVB	25298	40125	0.41%	0.110%
5	4.157	161	165	169	rVB2	12074	14126	0.15%	0.039%
6	4.734	260	263	269	rVB7	8260	12652	0.13%	0.035%
7	5.128	323	330	337	rBV	68002	111232	1.14%	0.305%
8	5.840	444	451	465	rBV5	24303	85062	0.88%	0.233%
9	7.251	684	691	709	rBV	108242	352974	3.63%	0.967%
10	7.387	709	714	732	rVB	168928	340027	3.50%	0.932%
11	7.592	743	749	764	rBV	204183	453642	4.67%	1.243%
12	8.063	820	829	850	rBV	500030	1018902	10.49%	2.793%
13	8.816	949	957	976	rBV2	46738	200951	2.07%	0.551%
14	9.263	1027	1033	1049	rBV	152775	392948	4.04%	1.077%
15	9.598	1087	1090	1096	rVB7	6677	10530	0.11%	0.029%
16	9.992	1150	1157	1176	rBV3	91935	330301	3.40%	0.905%
17	10.586	1251	1258	1280	rBV2	84236	375719	3.87%	1.030%
18	10.757	1285	1287	1293	rVB7	4597	9770	0.10%	0.027%
19	10.892	1302	1310	1327	rBV	551873	1263123	13.00%	3.462%
20	11.122	1343	1349	1351	rBV4	14447	28209	0.29%	0.077%
21	13.598	1765	1770	1774	rVB7	7109	11332	0.12%	0.031%
22	14.127	1854	1860	1874	rBV	346274	668263	6.88%	1.832%
23	14.410	1901	1908	1924	rBV	477564	841570	8.66%	2.307%
24	14.710	1953	1959	1971	rBV	857806	1475679	15.19%	4.045%
25	15.069	2015	2020	2023	rBV6	10446	21219	0.22%	0.058%
26	15.716	2123	2130	2145	rBV	527975	1013170	10.43%	2.777%
27	15.892	2155	2160	2179	rVB3	55365	188137	1.94%	0.516%
28	16.080	2187	2192	2201	rBV	177053	337082	3.47%	0.924%
29	16.521	2264	2267	2272	rBV7	9589	16792	0.17%	0.046%
30	16.639	2284	2287	2293	rBV	24607	30709	0.32%	0.084%
31	17.357	2405	2409	2412	rBV6	10339	17155	0.18%	0.047%
32	17.474	2423	2429	2441	rBV	992033	1651224	16.99%	4.526%
33	17.580	2441	2447	2462	rVB	478811	918750	9.46%	2.518%
34	18.268	2561	2564	2569	rBV2	69113	102680	1.06%	0.281%
35	18.321	2569	2573	2583	rVV	472244	735294	7.57%	2.015%
36	18.780	2648	2651	2663	rVB4	203536	552928	5.69%	1.516%

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37	19.410	2755	2758	2761	rBV3	65633	99057	1.02%	0.272%
38	19.551	2778	2782	2787	rBV	181829	259283	2.67%	0.711%
39	19.804	2820	2825	2838	rVB	822895	1415254	14.57%	3.879%
40	21.562	3119	3124	3132	rBV	1085559	1728903	17.79%	4.739%
41	22.933	3354	3357	3362	rVB2	258988	342523	3.53%	0.939%
42	23.245	3406	3410	3417	rVB	677350	1090109	11.22%	2.988%
43	23.333	3420	3425	3442	rVB4	471234	1514828	15.59%	4.152%
44	24.109	3551	3557	3571	rVB	813714	1957269	20.14%	5.365%
45	24.686	3649	3655	3663	rVB	1083383	2299782	23.67%	6.303%
46	26.650	3983	3989	3998	rBV	817417	2323237	23.91%	6.368%
47	28.791	4346	4353	4378	rVB2	2720099	9716301	100.00%	26.631%

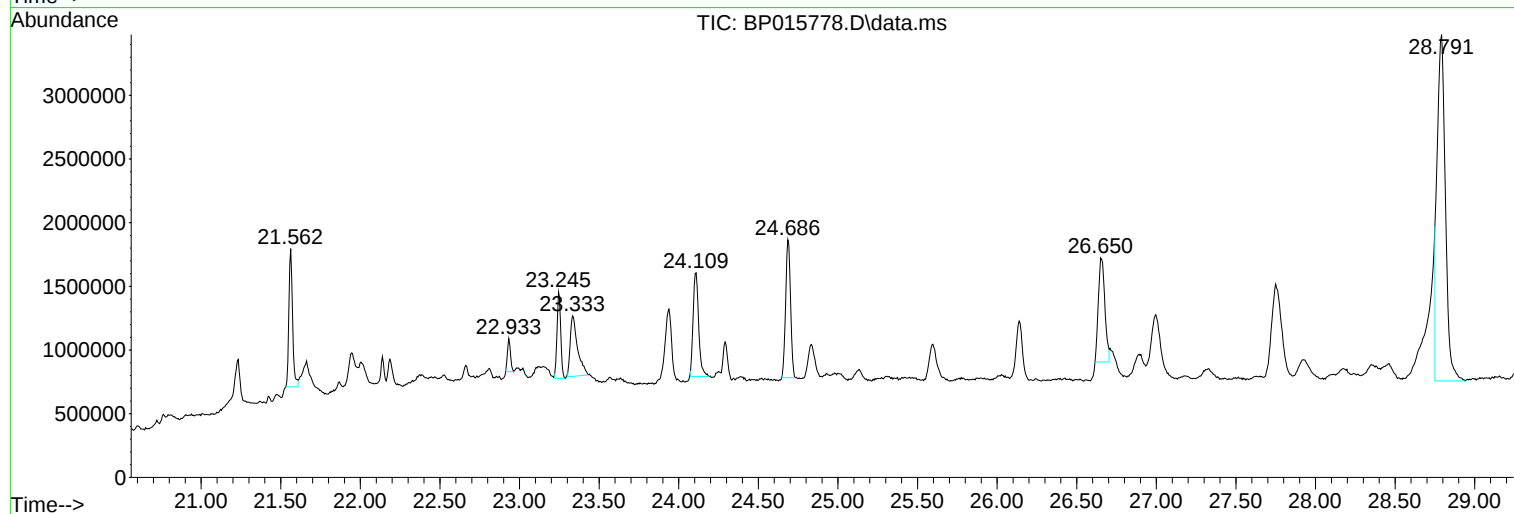
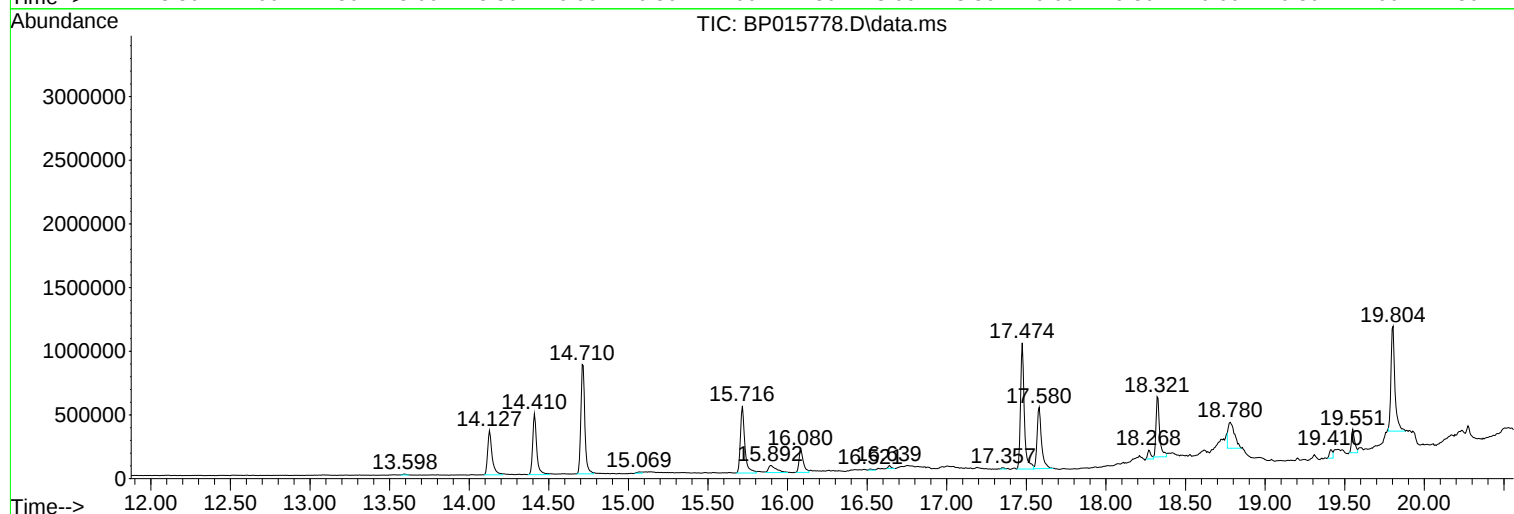
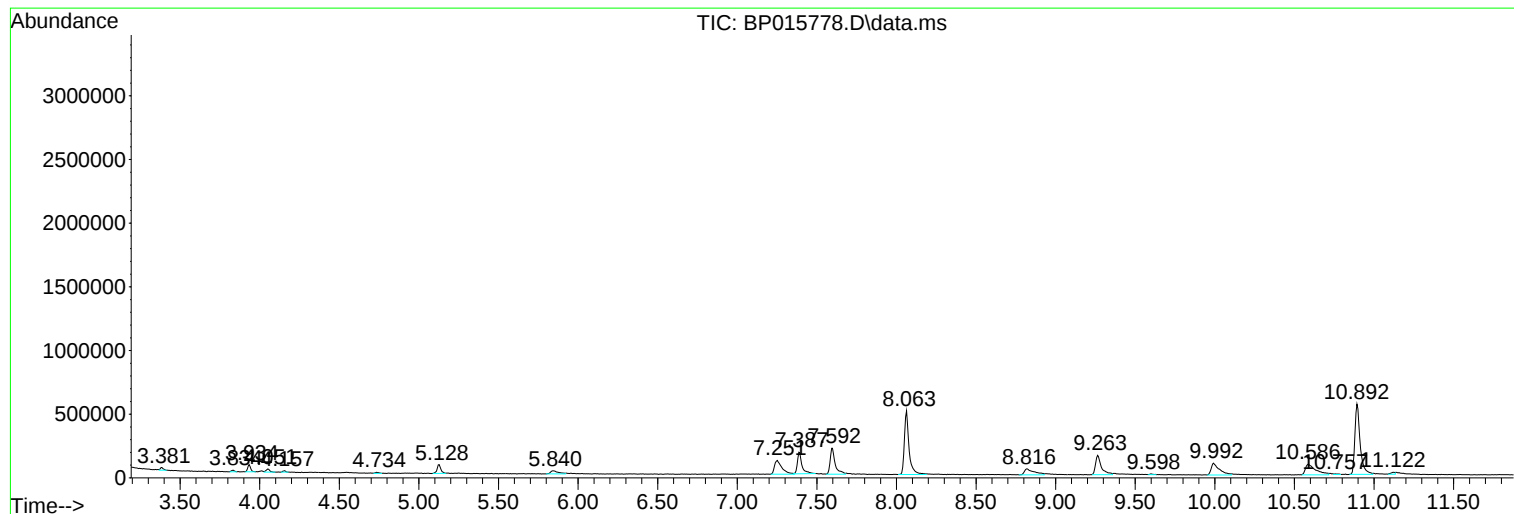
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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



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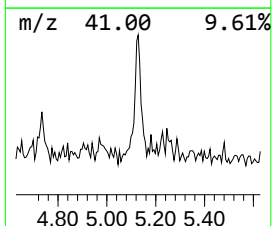
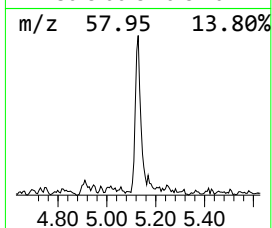
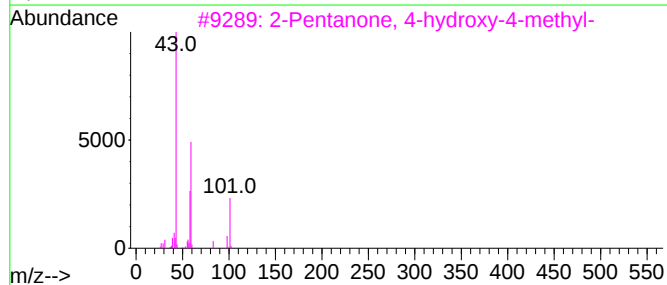
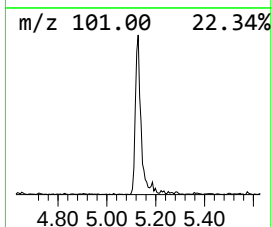
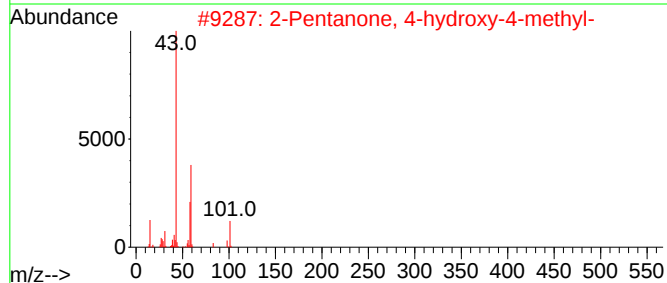
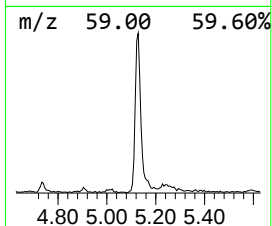
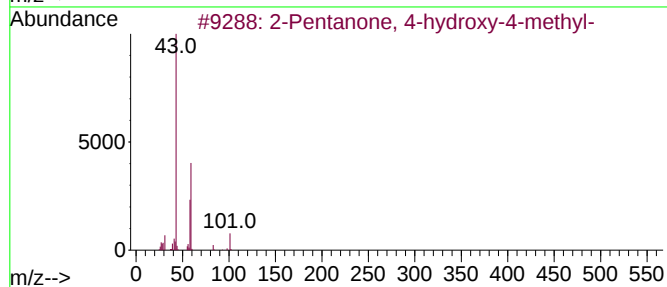
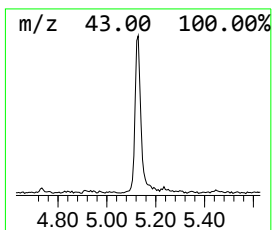
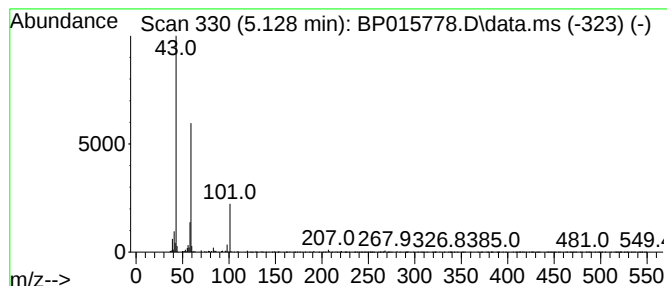
Instrument :
BNA_P
ClientSampleId :
DCFS0

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 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.128	2.18 ng/ul	111232	1,4-Dichlorobenzene-d4			8.063
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	45
3	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	45
4	3-Hexanol		102	C6H14O	000623-37-0	23
5	3-Pentanol, 2-methyl-		102	C6H14O	000565-67-3	17



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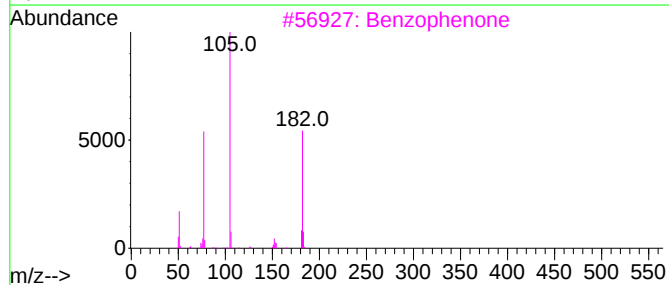
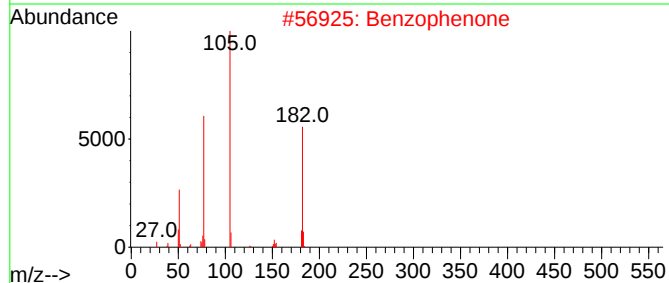
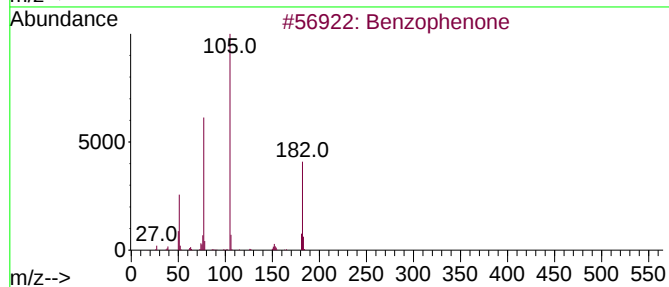
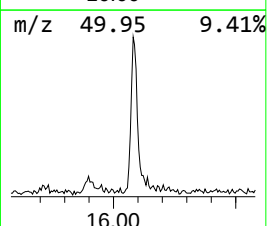
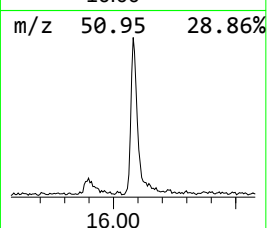
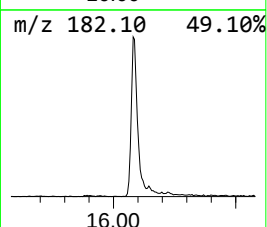
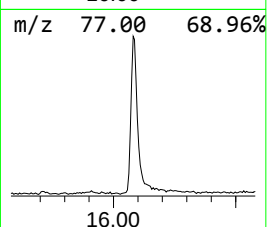
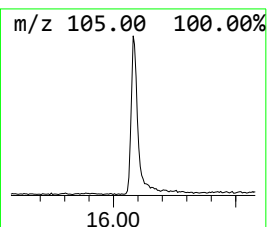
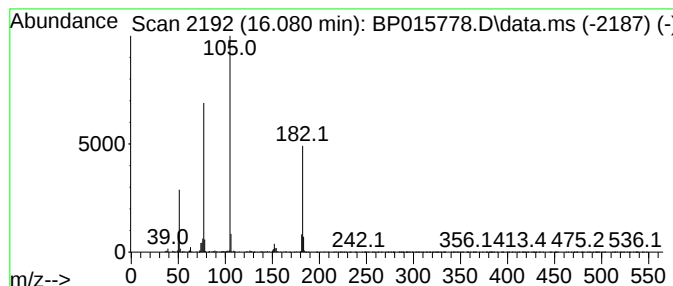
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	4.57 ng/ul	337082	Acenaphthene-d10	14.710

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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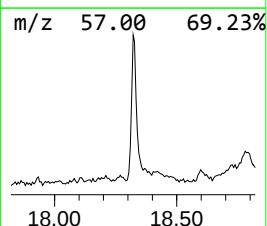
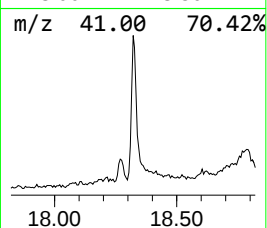
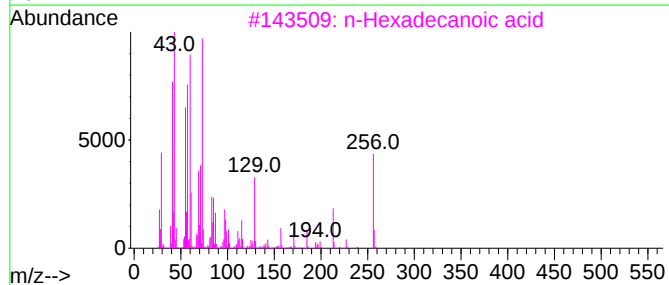
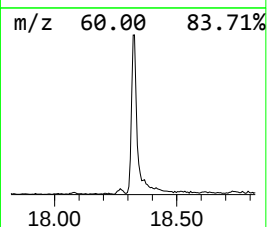
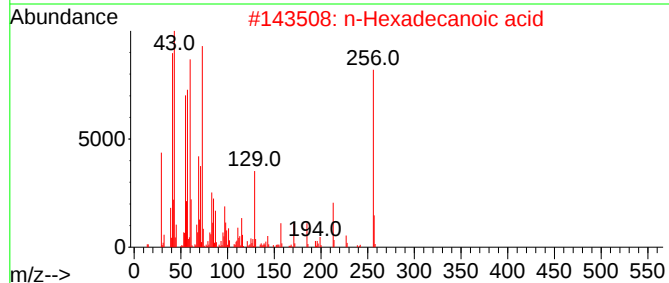
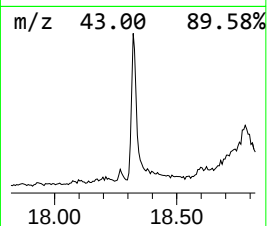
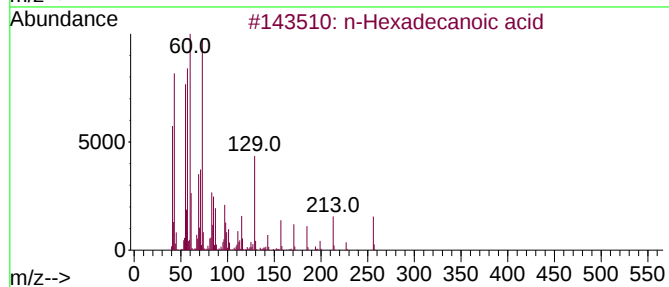
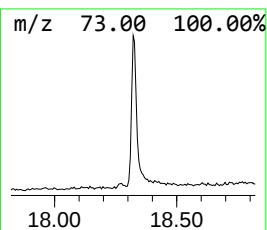
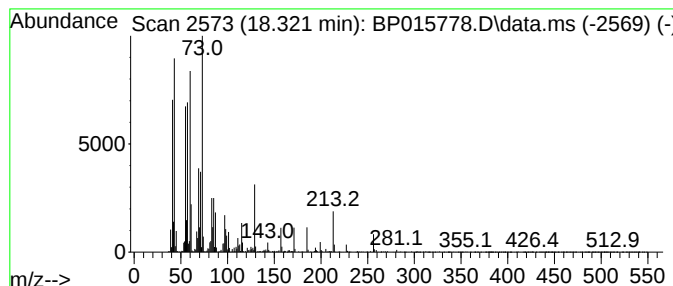
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.321	8.91 ng/ul	735294	Phenanthrene-d10	17.474

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	96
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91



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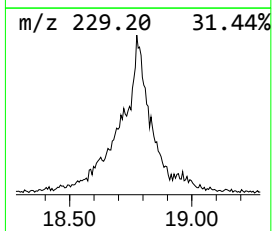
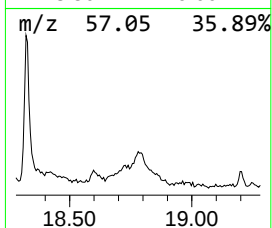
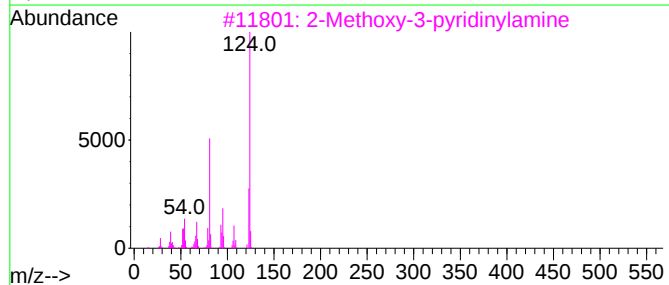
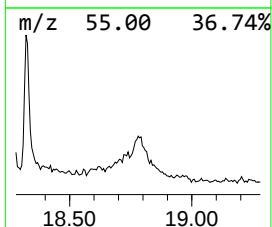
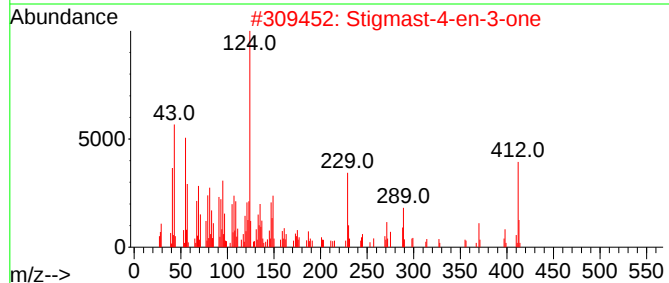
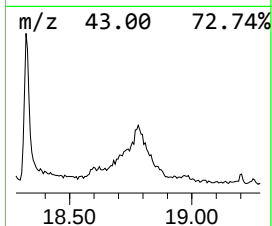
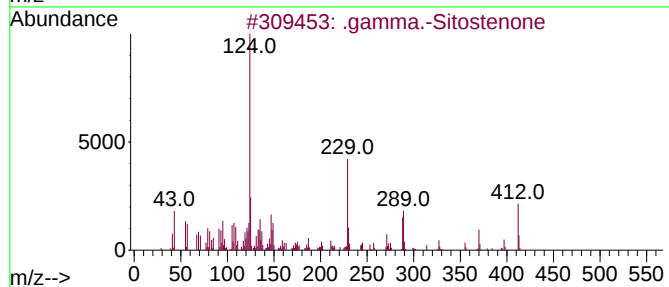
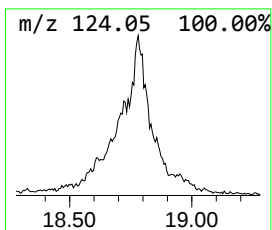
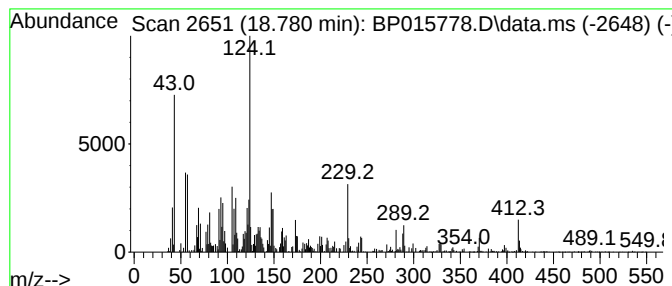
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 .gamma.-Sitostenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.780	6.70 ng/ul	552928	Phenanthrene-d10	17.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitostenone	412	C29H48O	084924-96-9	89
2			Stigmast-4-en-3-one	412	C29H48O	001058-61-3	46
3			2-Methoxy-3-pyridinylamine	124	C6H8N2O	1000484-55-0	46
4			2,4-Diaminophenol	124	C6H8N2O	000095-86-3	38
5			7.alpha.-Hydroxytestosterone	304	C19H28O3	000062-83-9	35



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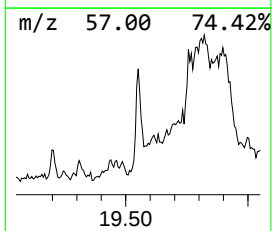
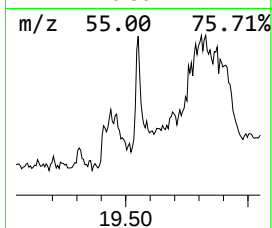
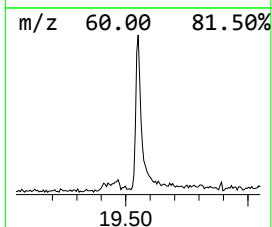
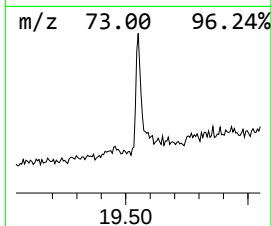
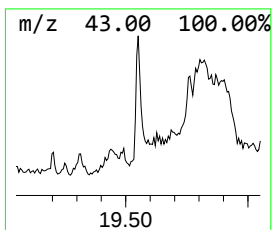
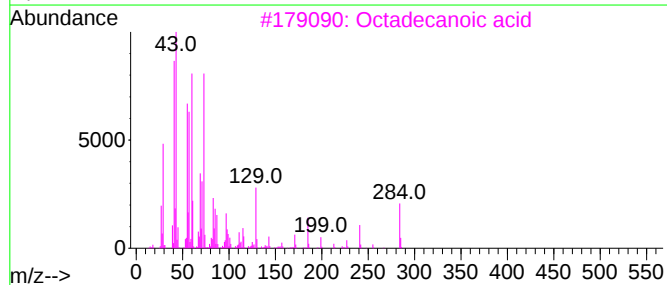
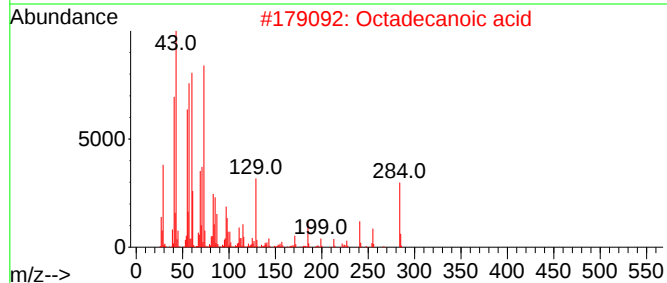
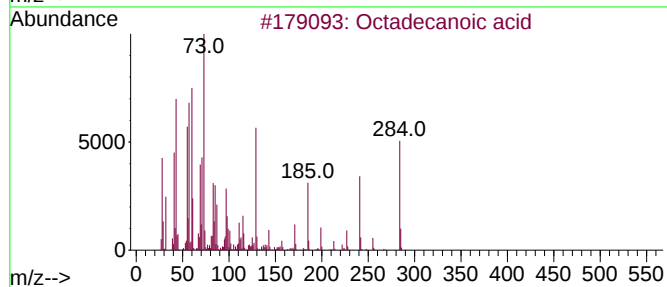
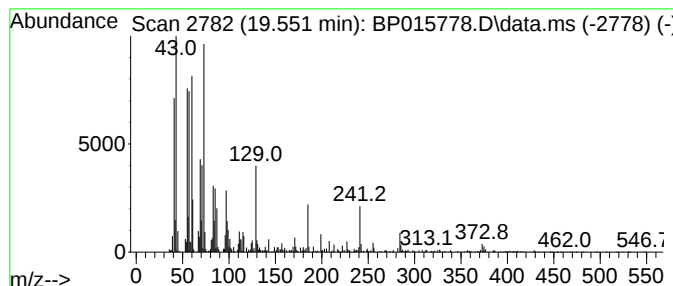
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	3.00 ng/ul	259283	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	95
5			Octadecanoic acid	284	C18H36O2	000057-11-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS0

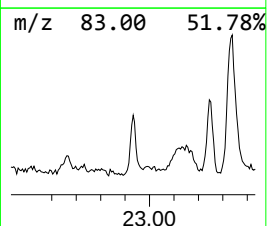
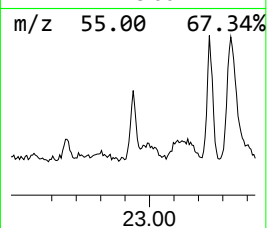
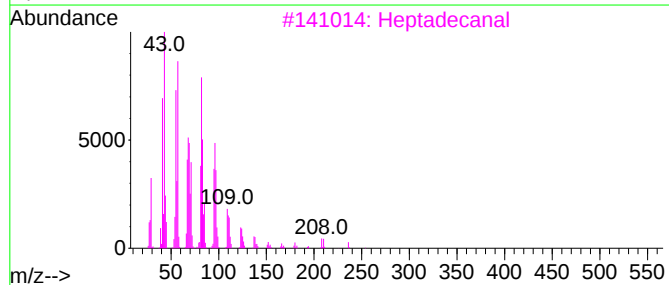
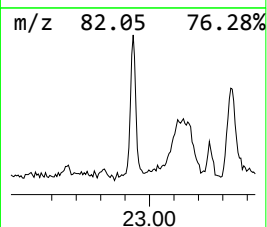
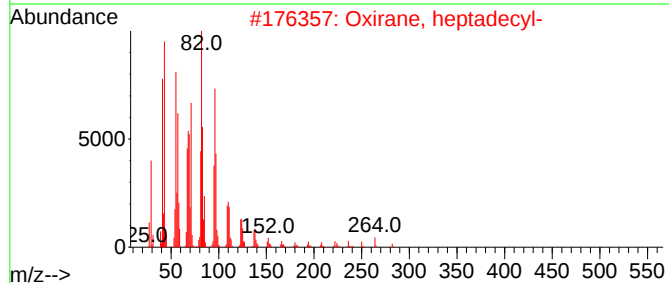
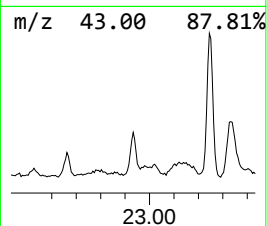
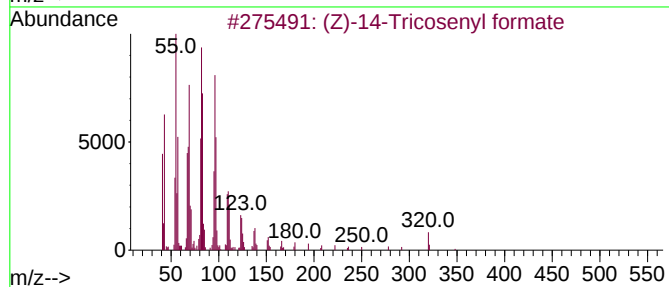
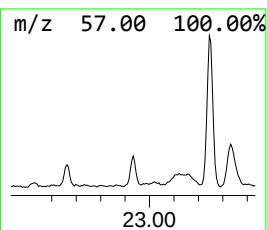
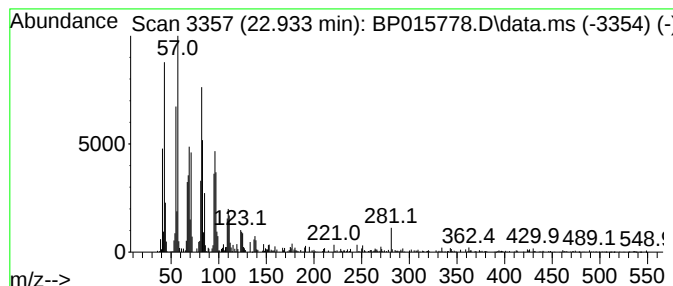
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (Z)-14-Tricosenyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.933	3.50 ng/ul	342523	Perylene-d12	24.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-14-Tricosenyl formate			366	C24H46O2	077899-10-6	95
2	Oxirane, heptadecyl-			282	C19H38O	067860-04-2	95
3	Heptadecanal			254	C17H34O	1000376-70-0	91
4	Octacosanal			408	C28H56O	022725-64-0	91
5	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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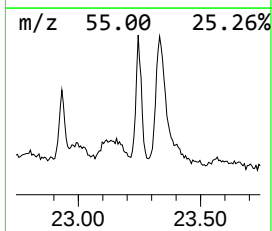
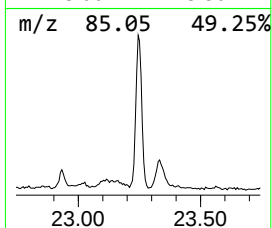
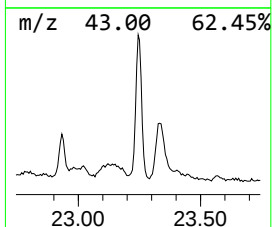
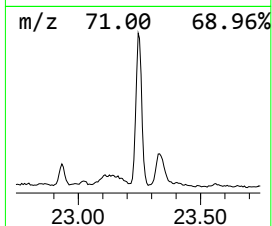
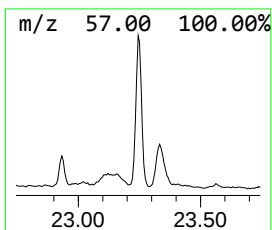
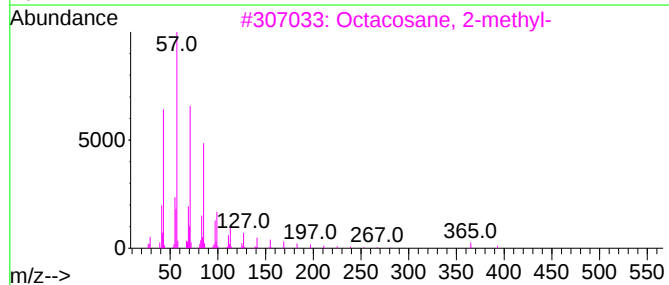
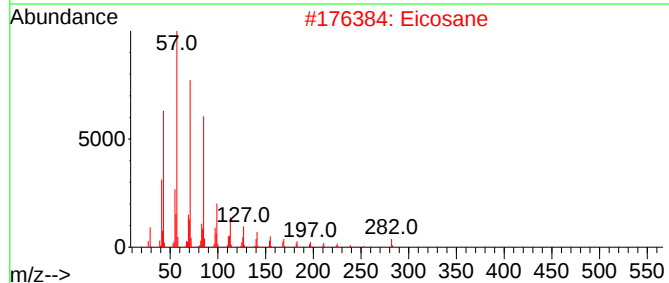
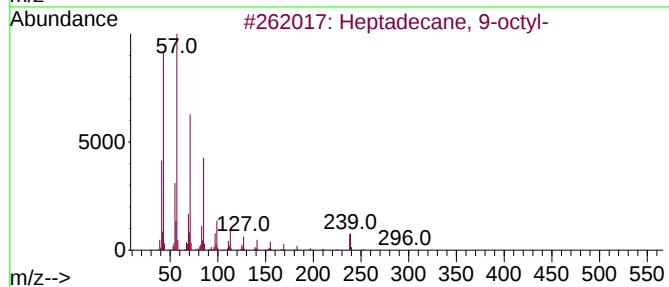
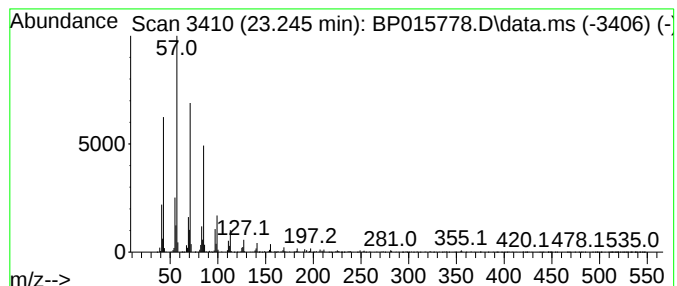
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.245	11.14 ng/ul	1090110	Perylene-d12	24.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	96
2			Eicosane	282	C20H42	000112-95-8	94
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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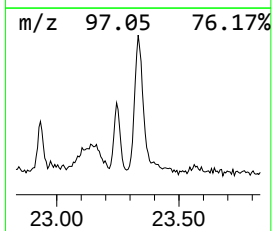
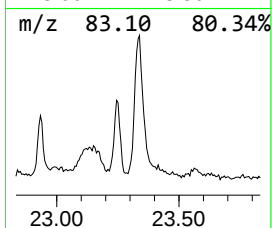
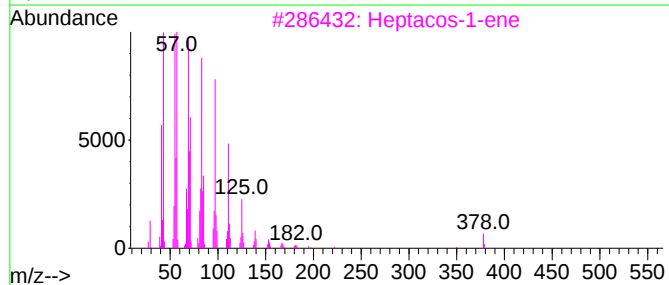
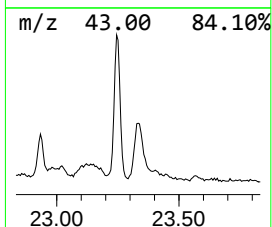
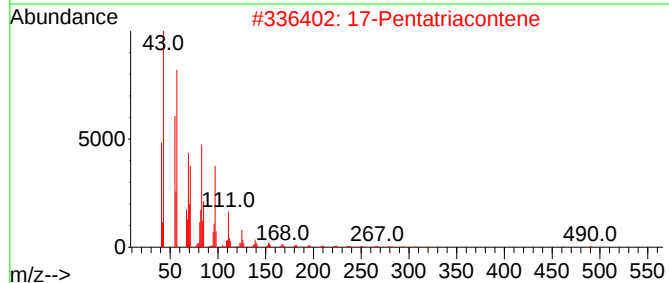
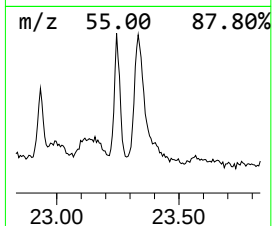
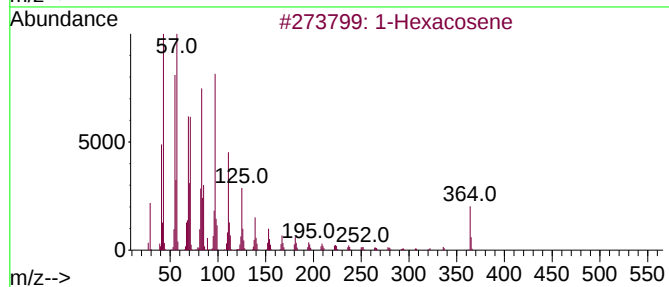
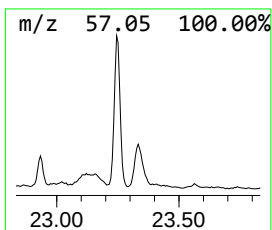
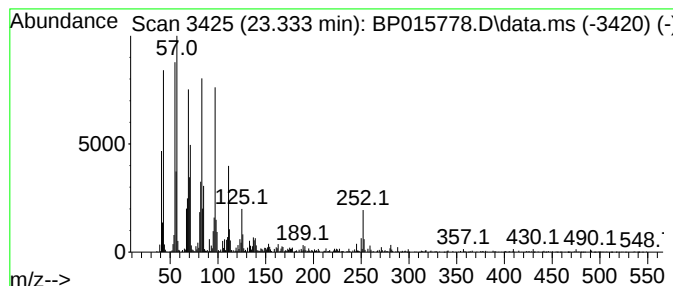
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.333	15.48 ng/ul	1514830	Perylene-d12	24.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	95
2	17-Pentatriacontene			491	C35H70	006971-40-0	94
3	Heptacos-1-ene			378	C27H54	015306-27-1	94
4	Pentacos-1-ene			350	C25H50	016980-85-1	94
5	Nonacos-1-ene			406	C29H58	018835-35-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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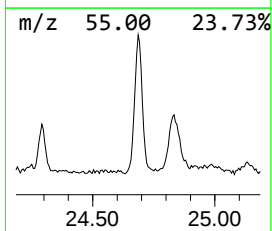
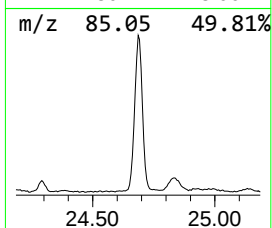
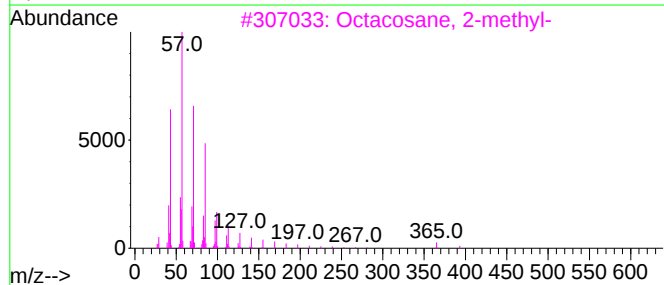
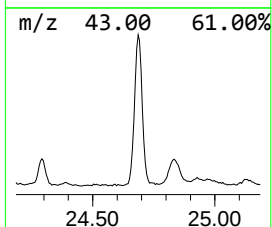
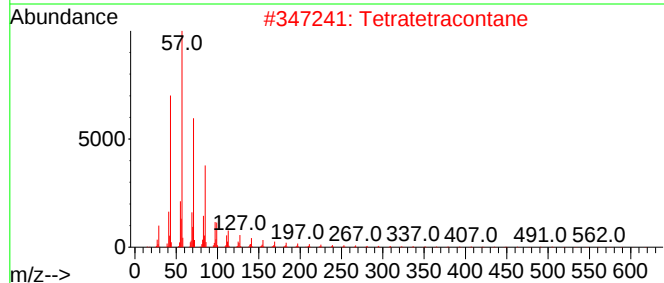
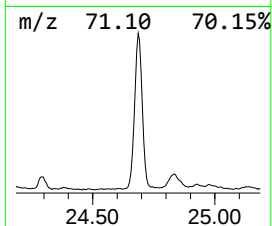
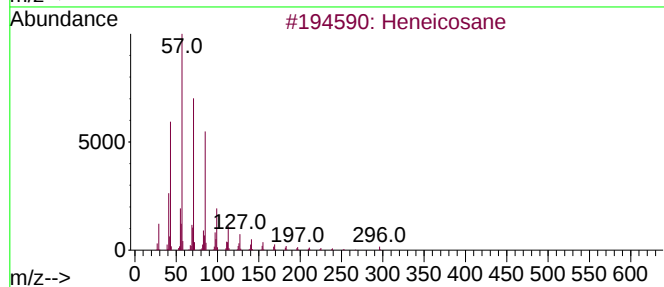
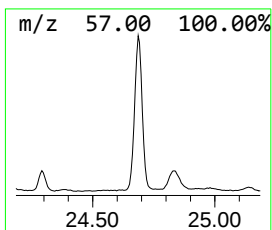
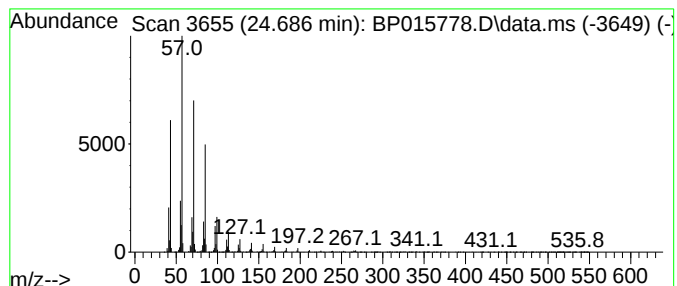
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.686	23.50 ng/ul	2299780	Perylene-d12	24.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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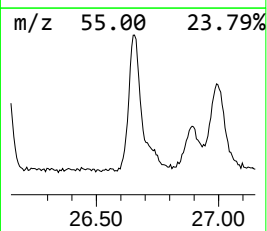
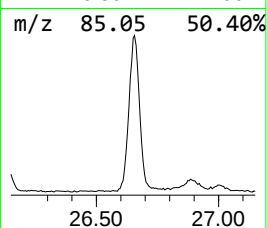
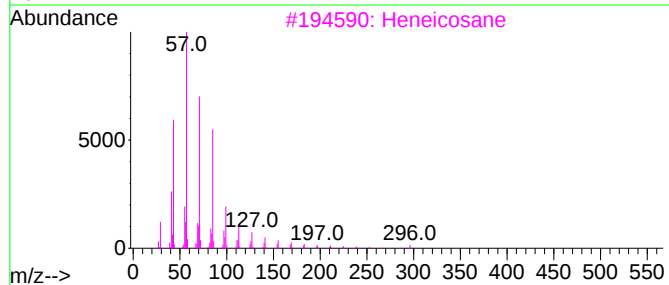
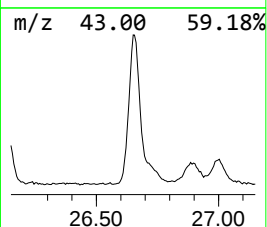
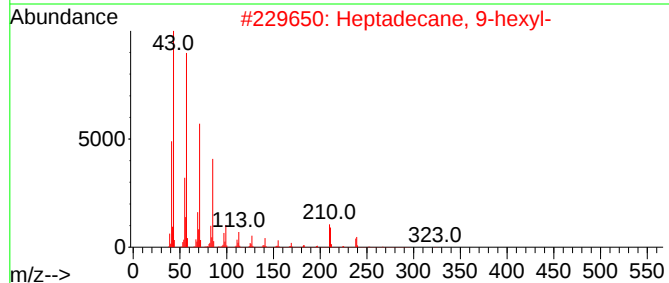
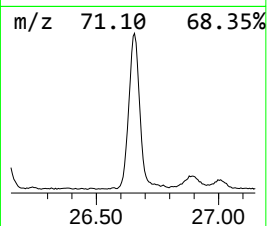
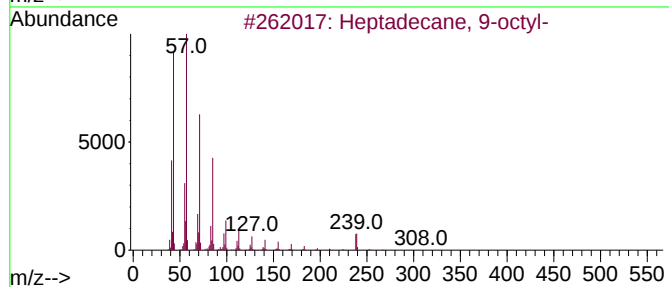
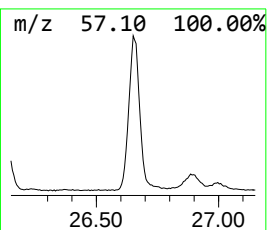
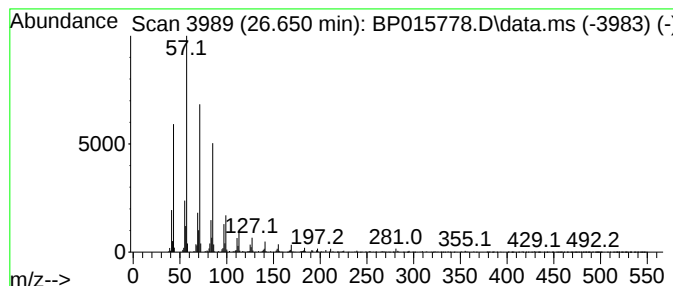
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.650	23.74 ng/ul	2323240	Perylene-d12	24.109

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
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Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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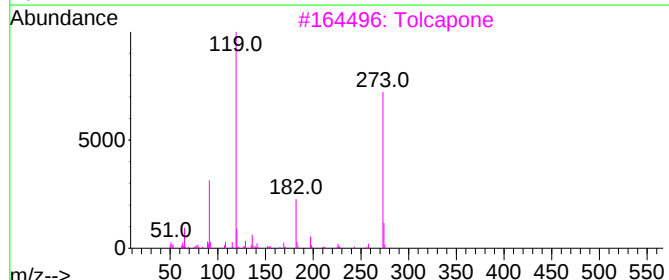
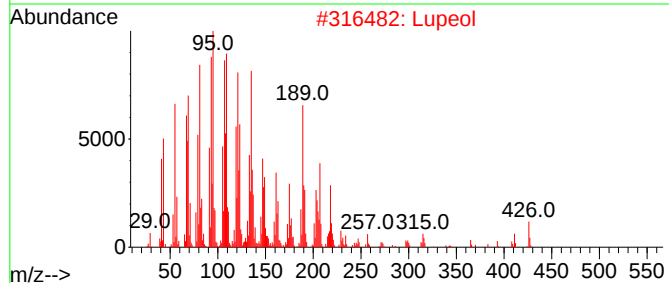
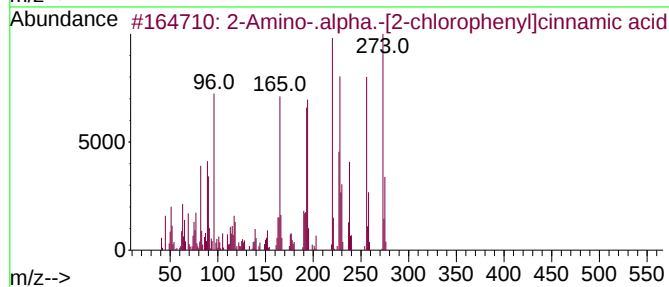
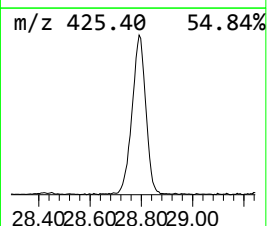
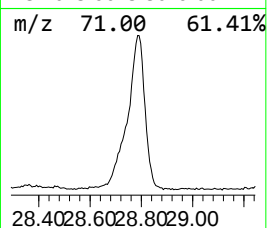
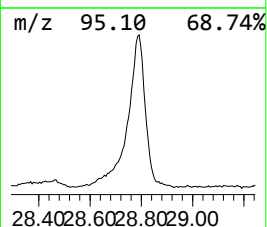
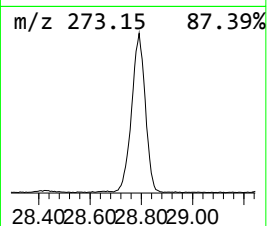
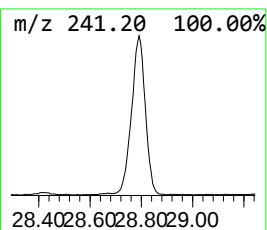
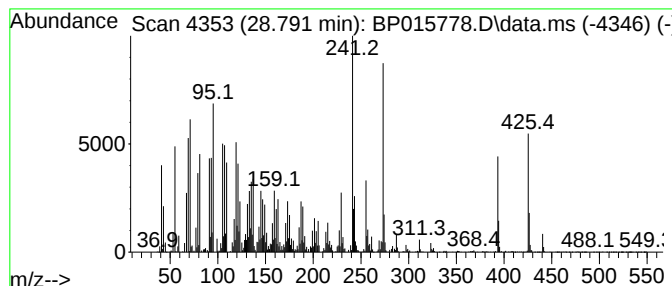
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.791	99.28 ng/ul	9716300	Perylene-d12	24.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2			Lupeol	426	C30H50O	000545-47-1	53
3			Tolcapone	273	C14H11NO5	134308-13-7	25
4			Phenol, 2,6-dimethyl-, phosphite...	394	C24H27O3P	052830-49-6	15
5			Pyrazolo[1,5-a]pyrimidine, 6,7-d...	273	C18H15N3	186956-30-9	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015778.D
Acq On : 28 Jun 2023 14:24
Operator : MA/JU
Sample : 03142-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS0

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
2-Pentanone, 4-...	5.128	2.2	ng/ul	111232	1	8.063	1018900	20.0
Benzophenone	16.080	4.6	ng/ul	337082	3	14.710	1475680	20.0
n-Hexadecanoic ...	18.321	8.9	ng/ul	735294	4	17.474	1651220	20.0
.gamma.-Sitoste...	18.780	6.7	ng/ul	552928	4	17.474	1651220	20.0
Octadecanoic acid	19.551	3.0	ng/ul	259283	5	21.562	1728900	20.0
(Z)-14-Tricosen...	22.933	3.5	ng/ul	342523	6	24.109	1957270	20.0
(DEL) Alkane: S...	23.245	11.1	ng/ul	1090110	6	24.109	1957270	20.0
(DEL) Alkane: S...	23.333	15.5	ng/ul	1514830	6	24.109	1957270	20.0
(DEL) Alkane: S...	24.686	23.5	ng/ul	2299780	6	24.109	1957270	20.0
(DEL) Alkane: S...	26.650	23.7	ng/ul	2323240	6	24.109	1957270	20.0
2-Amino-.alpha....	28.791	99.3	ng/ul	9716300	6	24.109	1957270	20.0