

Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
 Data File : BM012488.D
 Acq On : 27 Oct 2017 16:07
 Operator : SJ/JU
 Sample : I5873-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-13(1-3) 101117

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.098	163	172	182	rVB	5289271	7407072	1.08%	0.359%
2	5.410	386	395	401	rVB	16651115	25304982	3.68%	1.226%
3	5.557	411	420	428	rVB3	77036720	193713111	28.20%	9.384%
4	5.910	472	480	490	rVB2	45964429	71947795	10.47%	3.485%
5	12.845	1648	1659	1667	rBV	3829733	8460994	1.23%	0.410%
6	15.027	2012	2030	2044	rBV	24067016	81496757	11.86%	3.948%
7	16.856	2304	2341	2351	rBV2	103348884	686982290	100.00%	33.278%
8	17.304	2413	2417	2421	rVB	5930713	7963411	1.16%	0.386%
9	17.462	2440	2444	2453	rBV	4765689	6992728	1.02%	0.339%
10	18.450	2609	2612	2623	rVB	6963297	10066045	1.47%	0.488%
11	19.321	2754	2760	2761	rBV	12381928	17514766	2.55%	0.848%
12	19.397	2762	2773	2775	rBV2	45552236	139657481	20.33%	6.765%
13	19.533	2785	2796	2809	rVB	102024737	284121787	41.36%	13.763%
14	19.650	2813	2816	2819	rVV2	7712899	11678337	1.70%	0.566%
15	19.680	2819	2821	2830	rVB	7088494	8985532	1.31%	0.435%
16	20.456	2949	2953	2961	rVB2	13517452	22793486	3.32%	1.104%
17	20.562	2962	2971	2976	rBV2	23662320	43504607	6.33%	2.107%
18	21.139	3066	3069	3074	rVB	8786703	10369138	1.51%	0.502%
19	21.386	3100	3111	3115	rBV5	105914199	342056374	49.79%	16.569%
20	21.439	3115	3120	3124	rBV2	5666128	11233258	1.64%	0.544%
21	21.986	3209	3213	3218	rBV	33055304	42327933	6.16%	2.050%
22	26.962	4053	4059	4065	rBV2	5305453	13228094	1.93%	0.641%
23	27.044	4068	4073	4081	rVB3	6629716	16583986	2.41%	0.803%

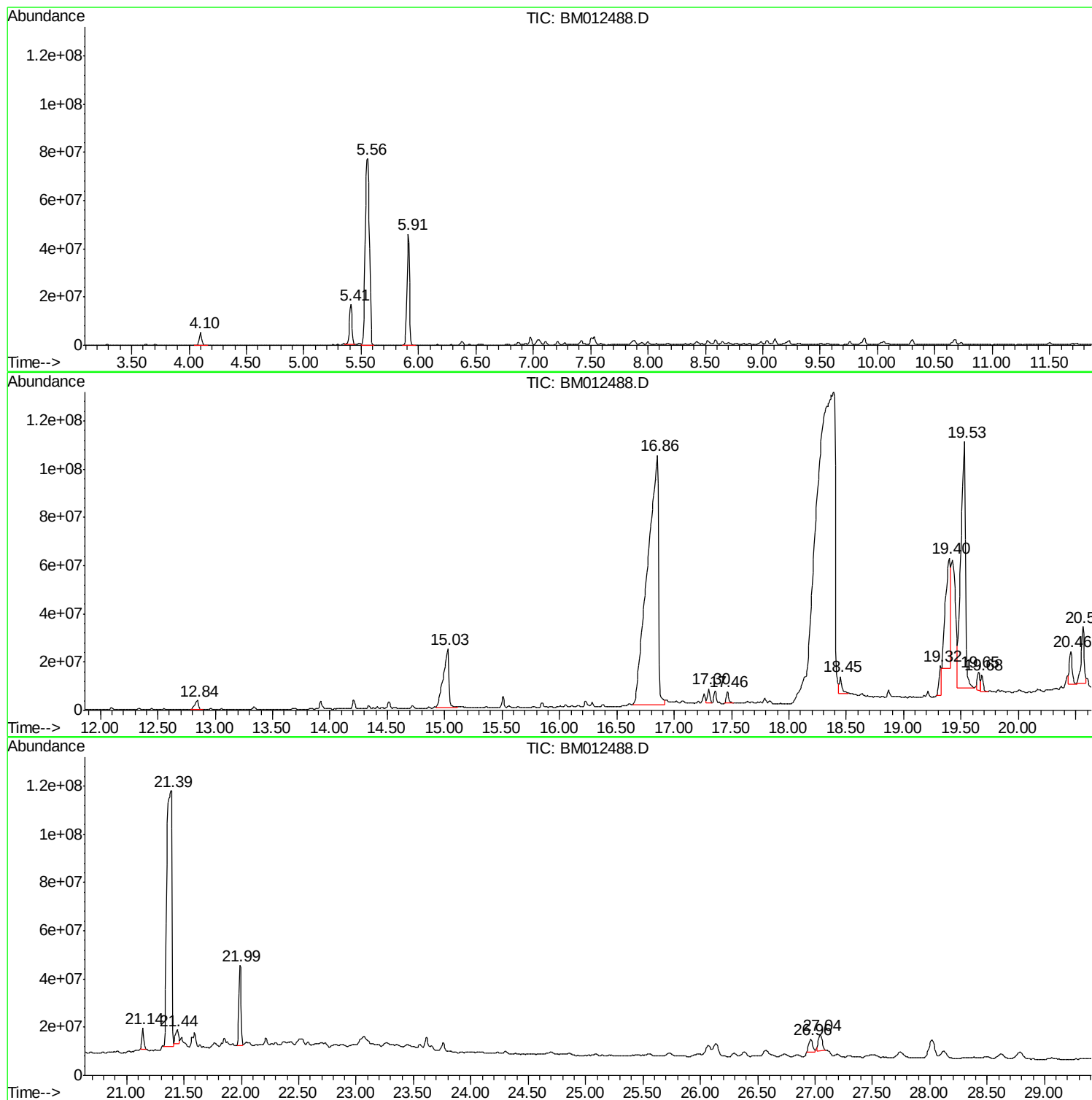
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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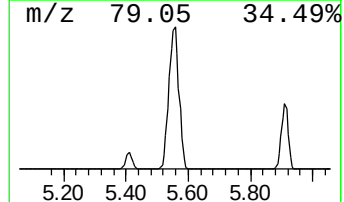
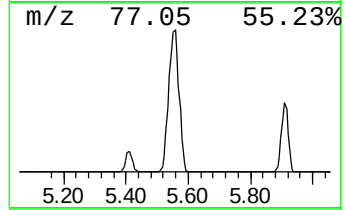
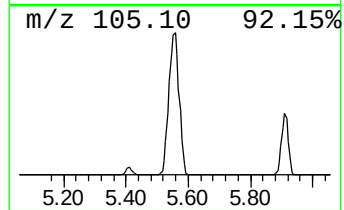
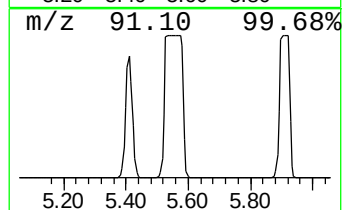
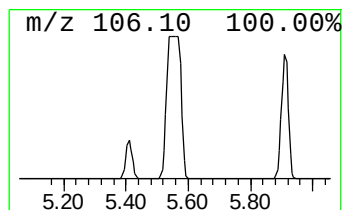
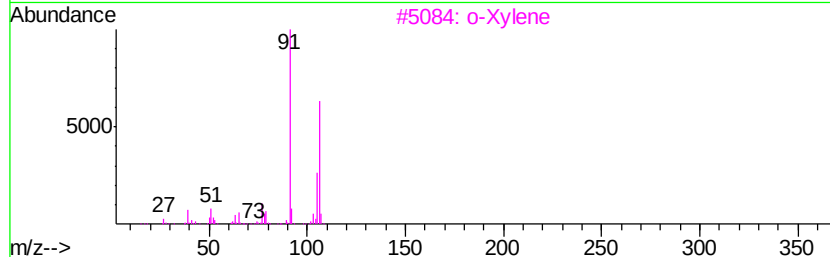
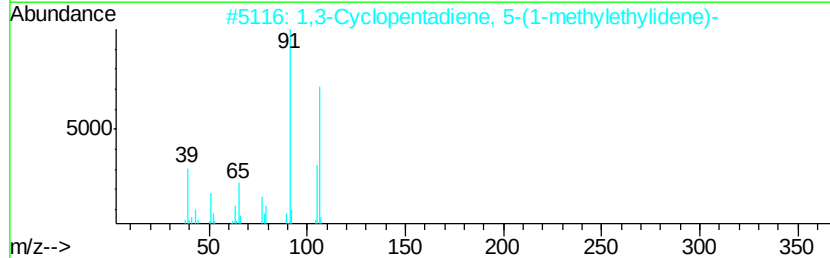
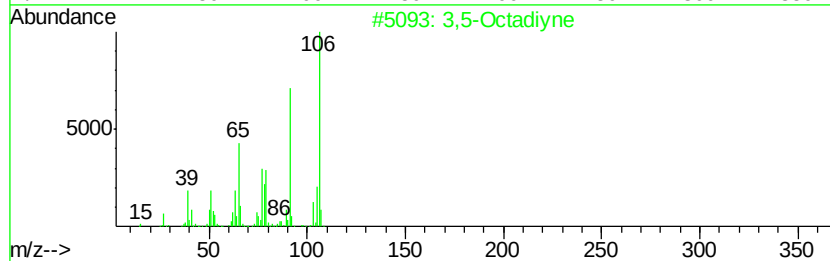
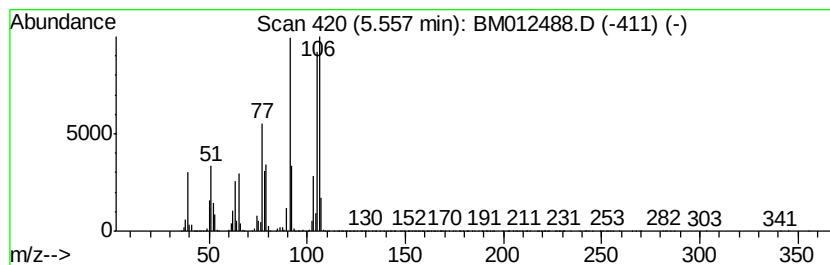
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3,5-Octadiyne Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	53.85 ng/ul	193713000	1,4-Dichlorobenzene-d4	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Octadiyne	106	C8H10	016387-70-5	68
2		1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	68
3		o-Xylene	106	C8H10	000095-47-6	59
4		p-Xylene	106	C8H10	000106-42-3	53
5		1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	53



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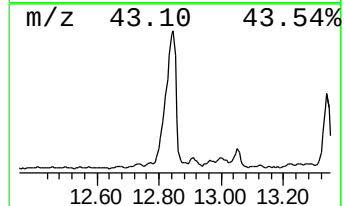
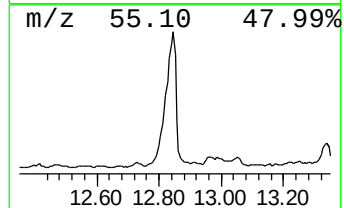
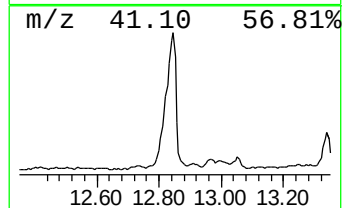
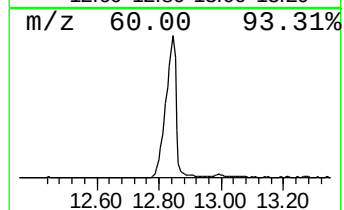
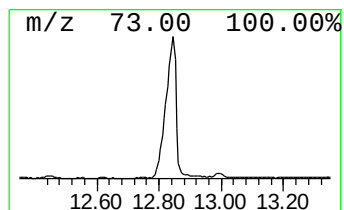
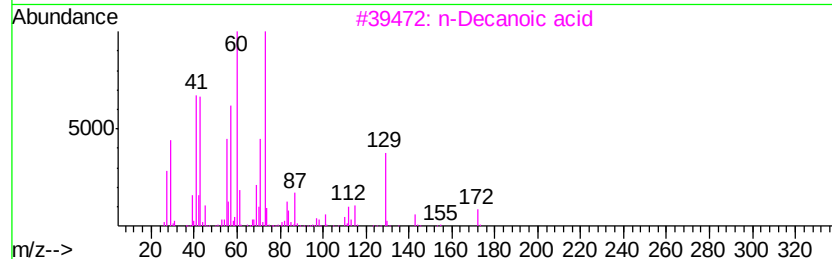
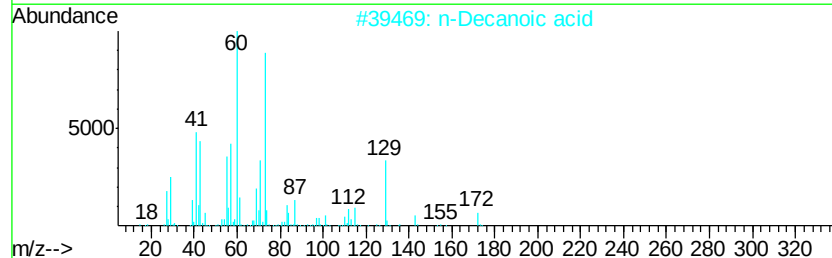
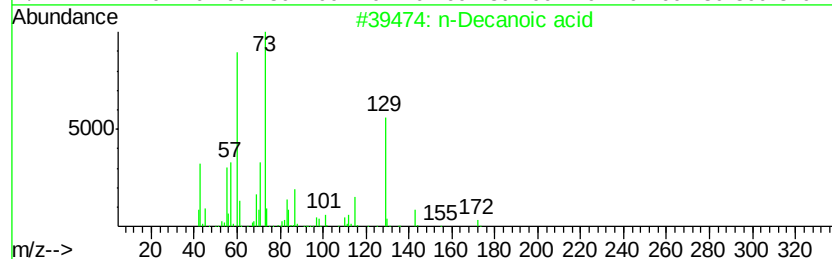
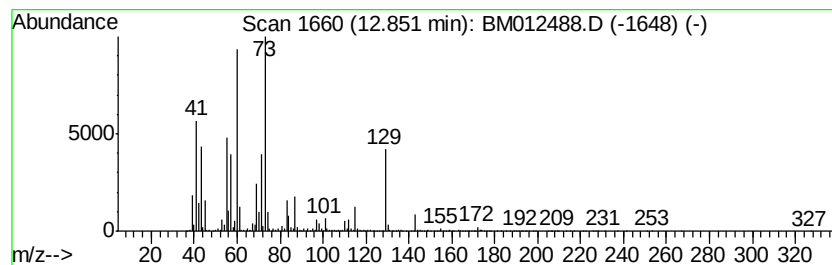
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Peak Number 5 n-Decanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.08 ng/ul	8460990	Acenaphthene-d10	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Decanoic acid	172 C10H20O2	000334-48-5	97
2	n-Decanoic acid	172 C10H20O2	000334-48-5	94
3	n-Decanoic acid	172 C10H20O2	000334-48-5	94
4	n-Decanoic acid	172 C10H20O2	000334-48-5	86
5	n-Decanoic acid	172 C10H20O2	000334-48-5	55



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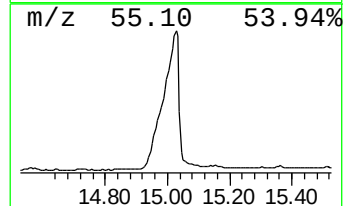
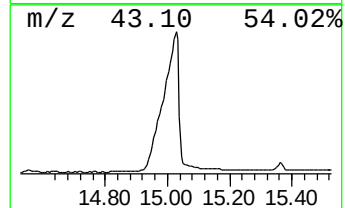
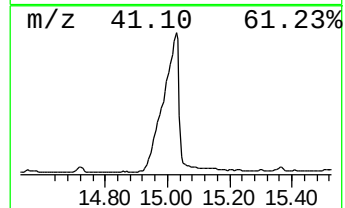
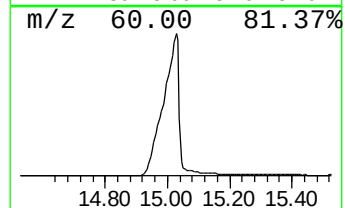
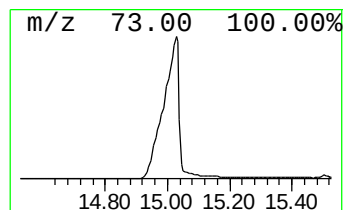
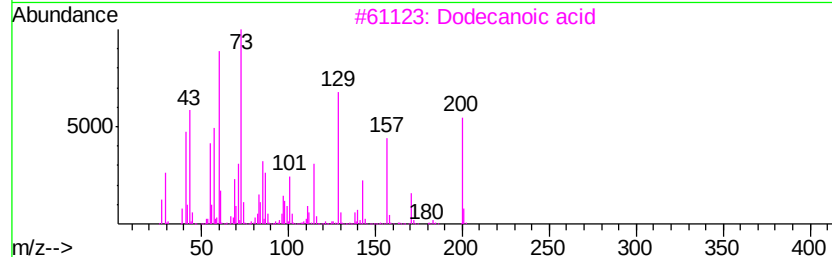
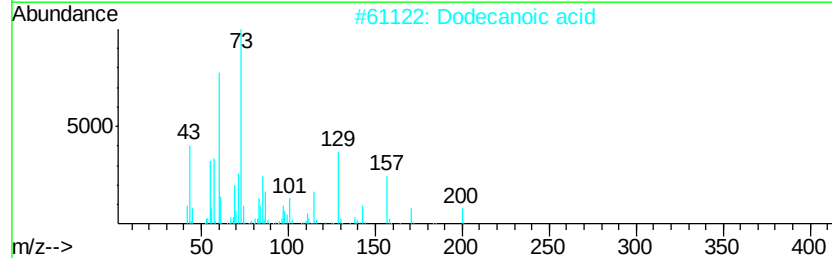
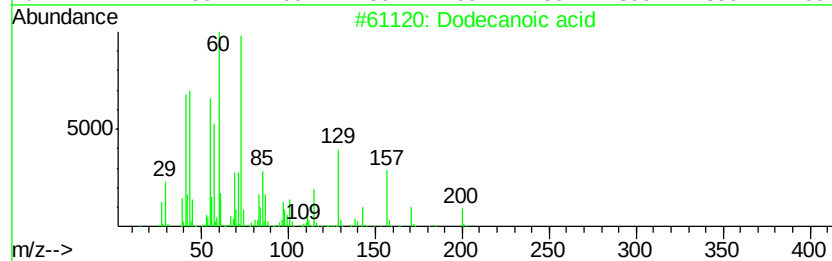
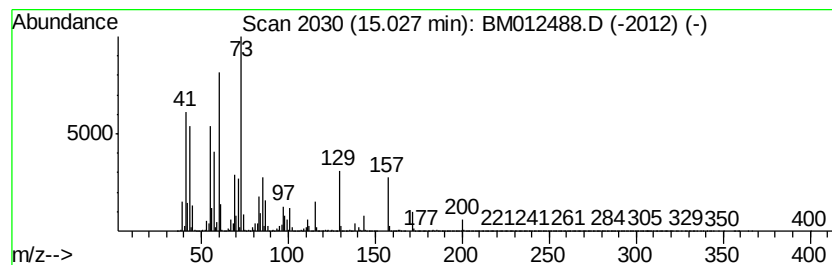
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Peak Number 6 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	20.00 ng/ul	81496800	Acenaphthene-d10	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid	200 C12H24O2	000143-07-7	98
2	Dodecanoic acid	200 C12H24O2	000143-07-7	98
3	Dodecanoic acid	200 C12H24O2	000143-07-7	94
4	Dodecanoic acid	200 C12H24O2	000143-07-7	91
5	Dodecanoic acid	200 C12H24O2	000143-07-7	91



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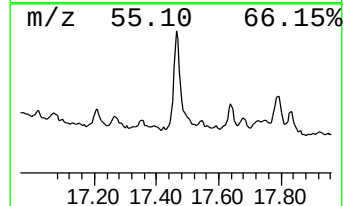
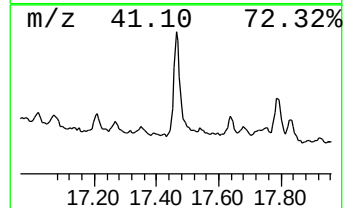
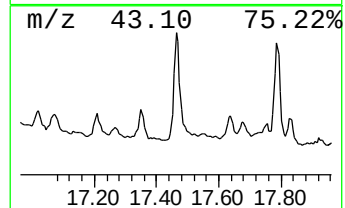
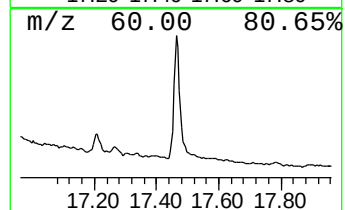
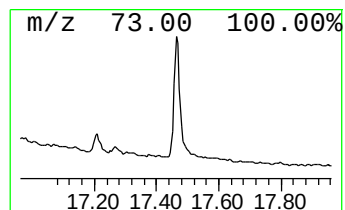
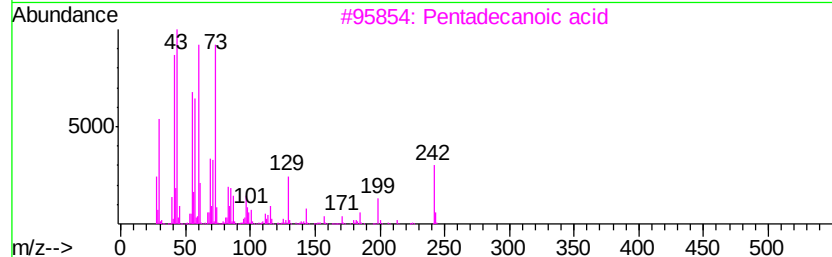
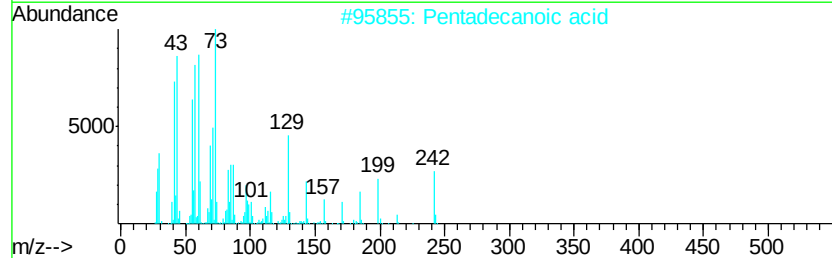
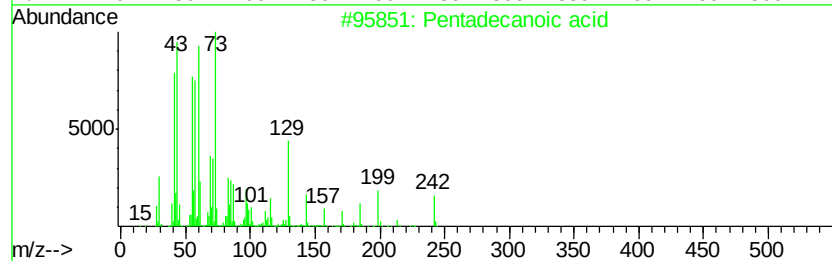
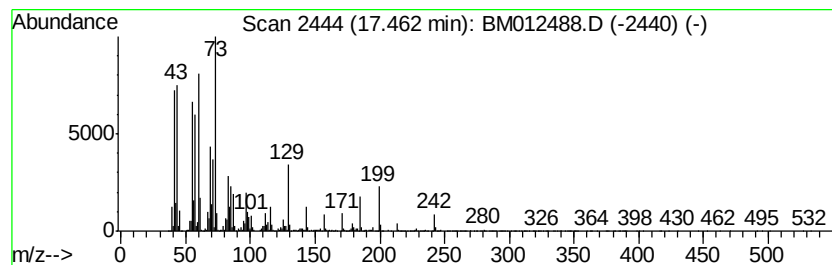
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Pentadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	17.56 ng/ul	6992730	Phenanthrene-d10	17.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	98
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	95
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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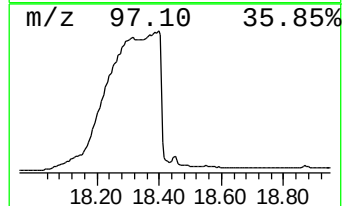
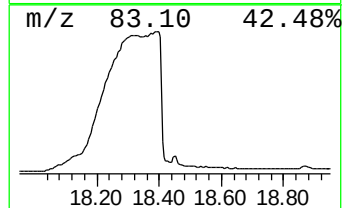
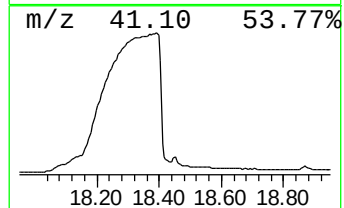
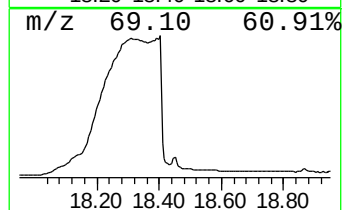
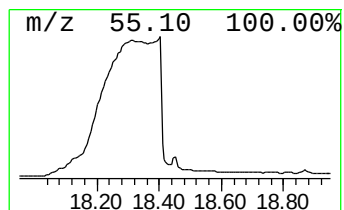
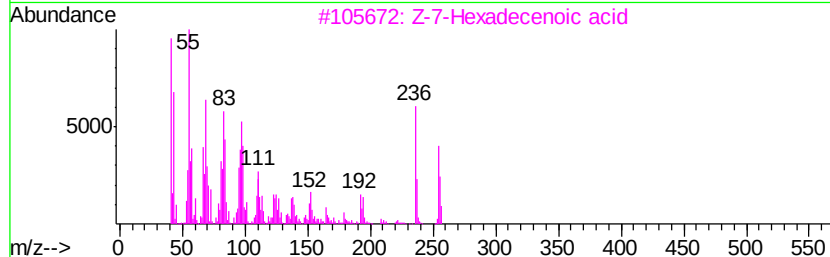
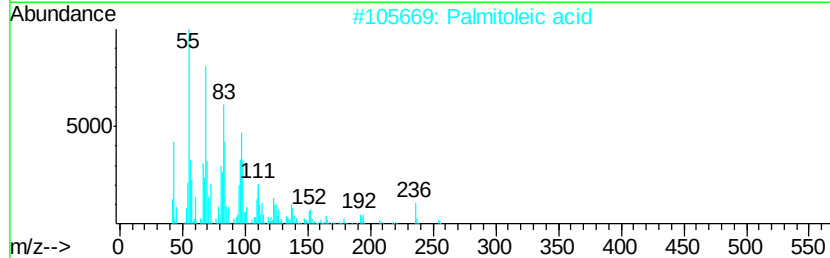
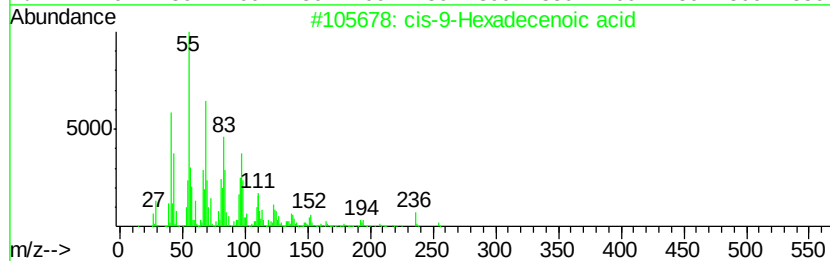
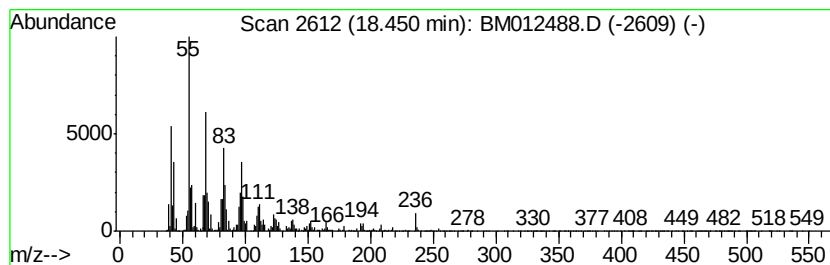
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Peak Number 8 cis-9-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.45	25.28 ng/ul	10066000	Phenanthrene-d10	17.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	98
2		Palmitoleic acid	254	C16H30O2	000373-49-9	96
3		Z-7-Hexadecenoic acid	254	C16H30O2	1000130-90-8	92
4		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	91
5		9-Hexadecenoic acid	254	C16H30O2	002091-29-4	90



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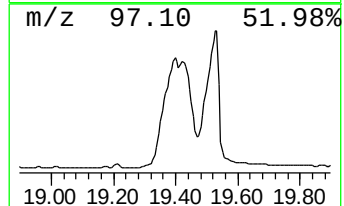
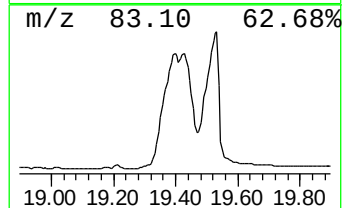
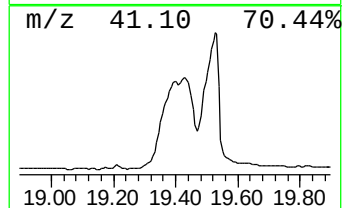
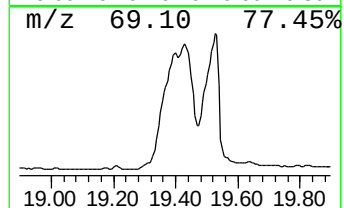
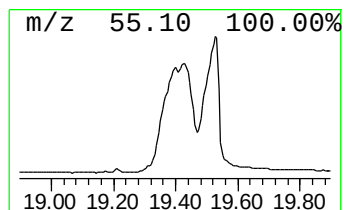
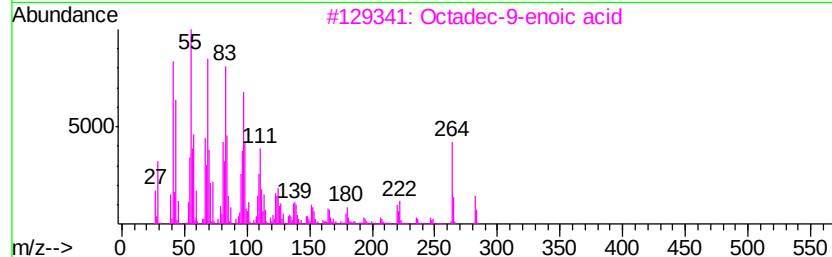
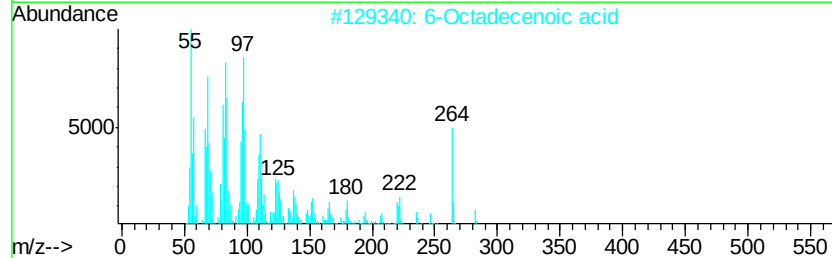
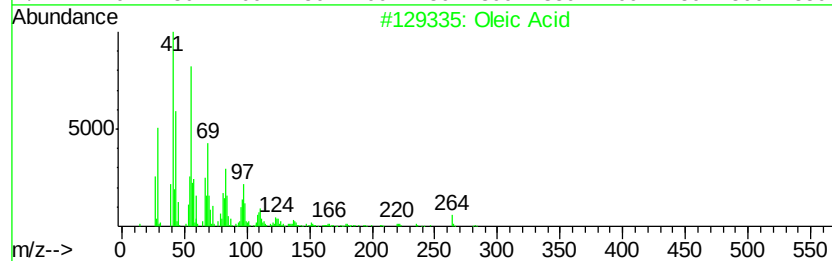
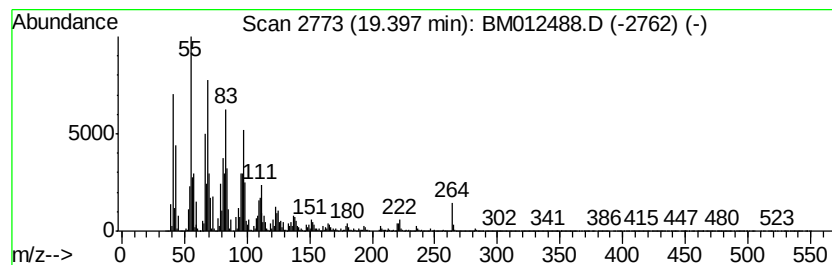
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Oleic Acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.40	248.65 ng/ul	139657000	Chrysene-d12	21.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oleic Acid	282	C18H34O2	000112-80-1	97
2		6-Octadecenoic acid	282	C18H34O2	1000336-66-8	95
3		Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	90
4		cis-Vaccenic acid	282	C18H34O2	000506-17-2	89
5		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	83



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
Data File : BM012488.D
Acq On : 27 Oct 2017 16:07
Operator : SJ/JU
Sample : I5873-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-13(1-3) 101117

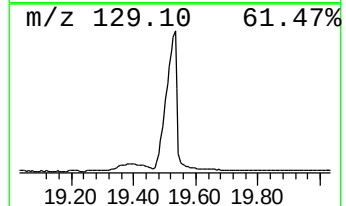
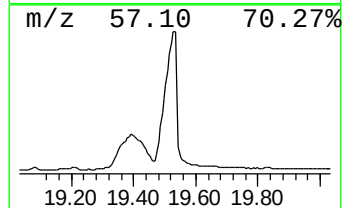
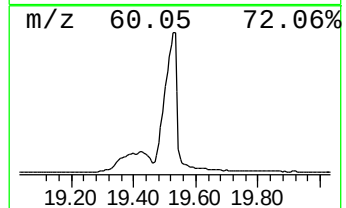
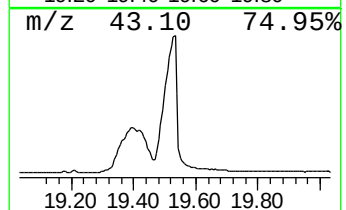
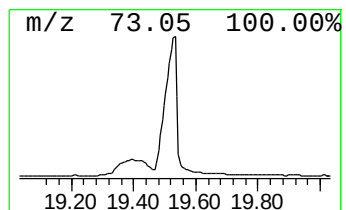
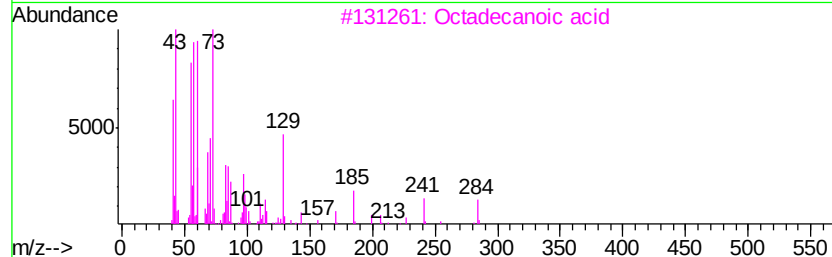
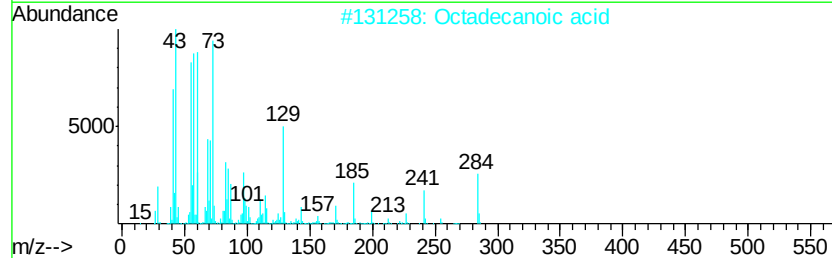
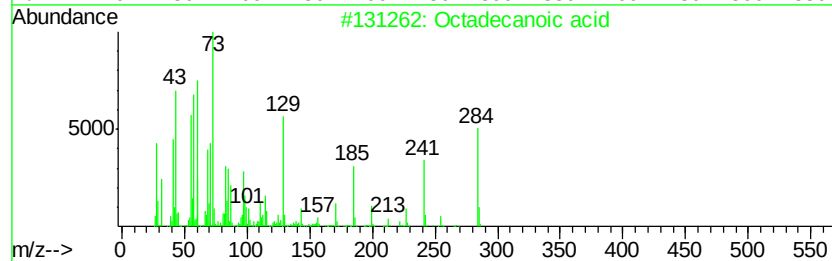
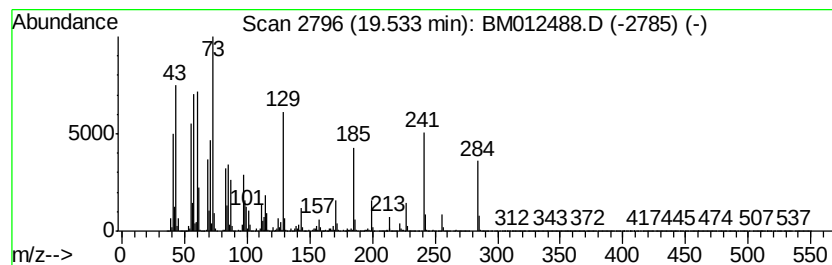
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.53	505.86 ng/ul	284122000	Chrysene-d12	21.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	99
3		Octadecanoic acid	284	C18H36O2	000057-11-4	99
4		Octadecanoic acid	284	C18H36O2	000057-11-4	98
5		Octadecanoic acid	284	C18H36O2	000057-11-4	93



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
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Operator : SJ/JU
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Misc :
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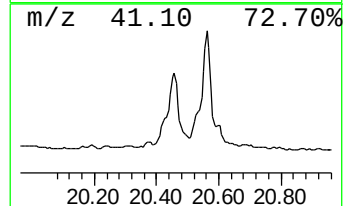
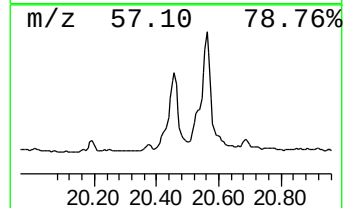
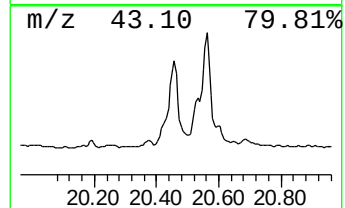
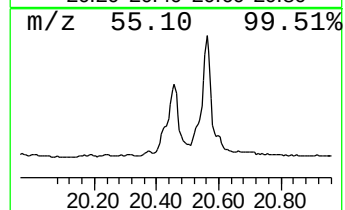
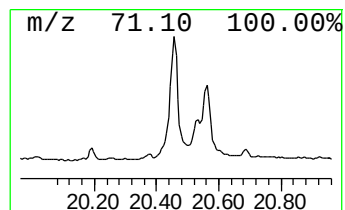
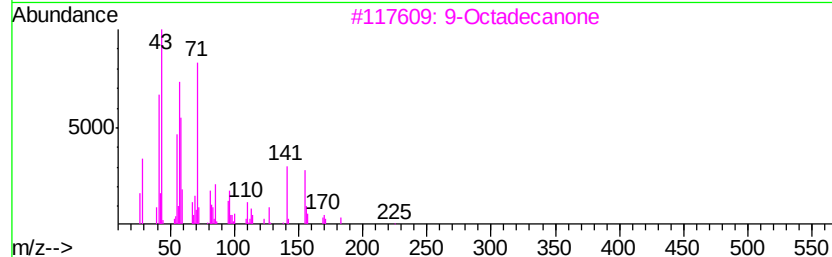
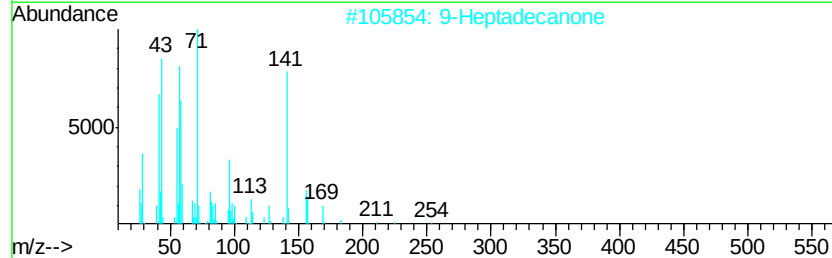
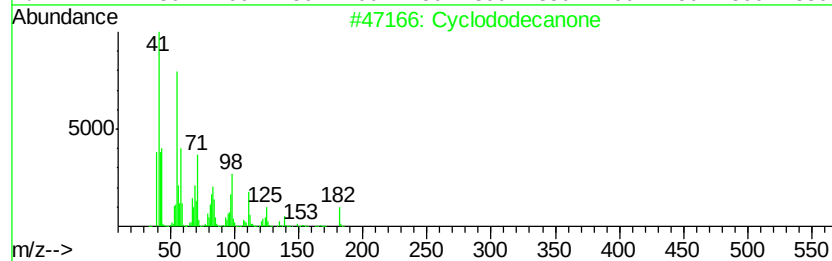
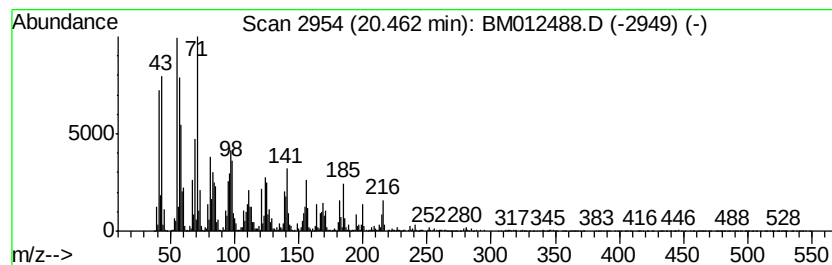
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	40.58 ng/ul	22793500	Chrysene-d12	21.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclododecanone	182	C12H22O	000830-13-7	38
2		9-Heptadecanone	254	C17H34O	000540-08-9	38
3		9-Octadecanone	268	C18H36O	018394-00-8	38
4		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	35
5		Cyclododecanone	182	C12H22O	000830-13-7	30



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
Data File : BM012488.D
Acq On : 27 Oct 2017 16:07
Operator : SJ/JU
Sample : I5873-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-13(1-3)_101117

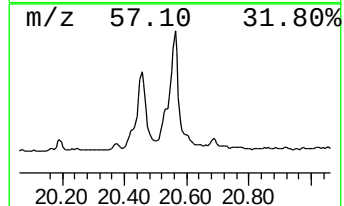
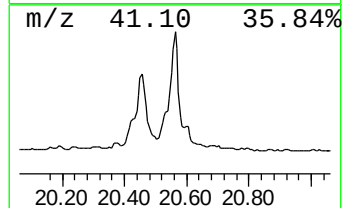
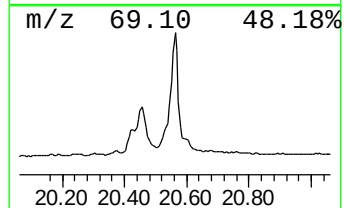
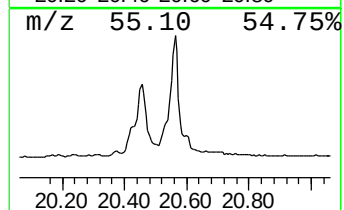
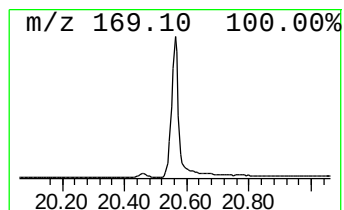
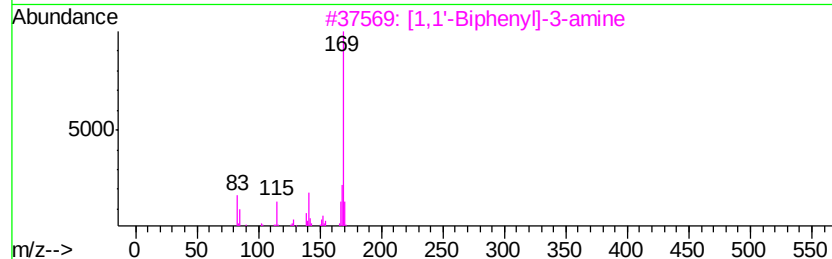
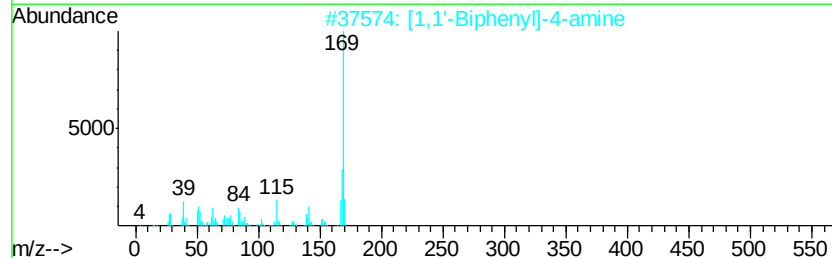
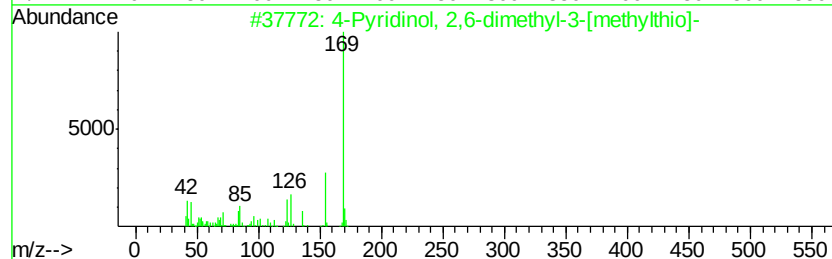
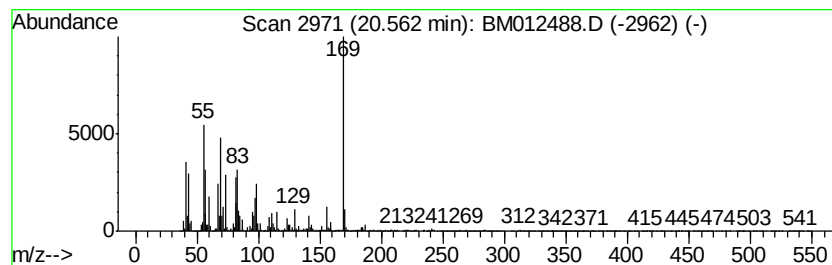
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	77.46 ng/ul	43504600	Chrysene-d12	21.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Pyridinol, 2,6-dimethyl-3-[met...	169	C8H11NOS	1000251-72-8	43
2		[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	38
3		[1,1'-Biphenyl]-3-amine	169	C12H11N	002243-47-2	38
4		7-Hydroxyimino-4,5,6,7-tetrahydr...	169	C6H7N3O3	1000110-77-2	38
5		Fumaric acid, 3-heptyl pentyl ester	284	C16H28O4	1000348-68-1	38



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
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Acq On : 27 Oct 2017 16:07
Operator : SJ/JU
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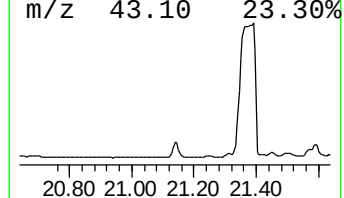
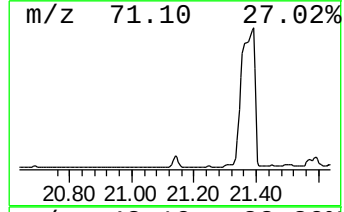
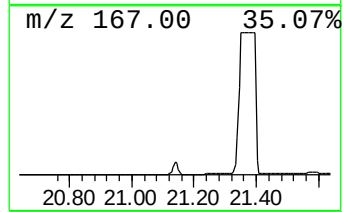
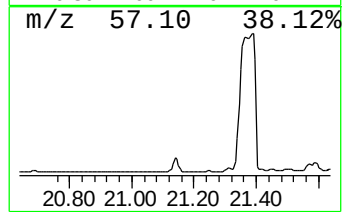
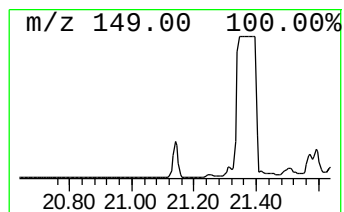
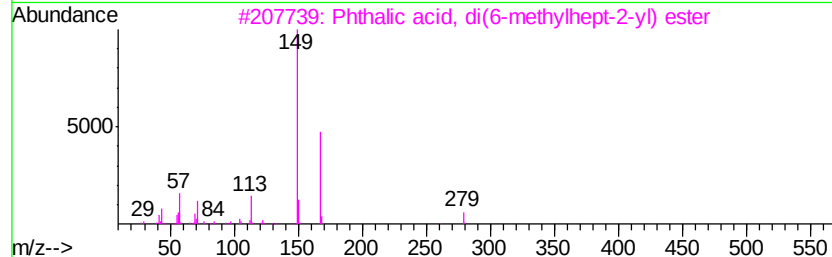
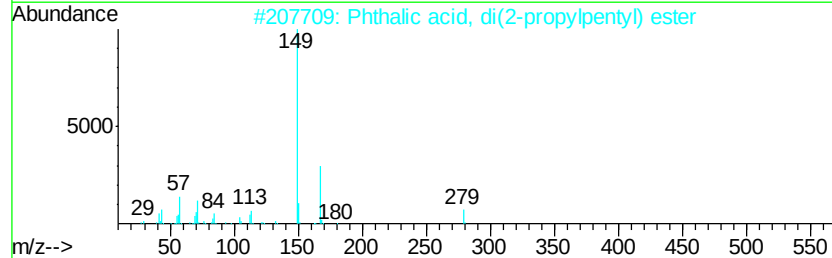
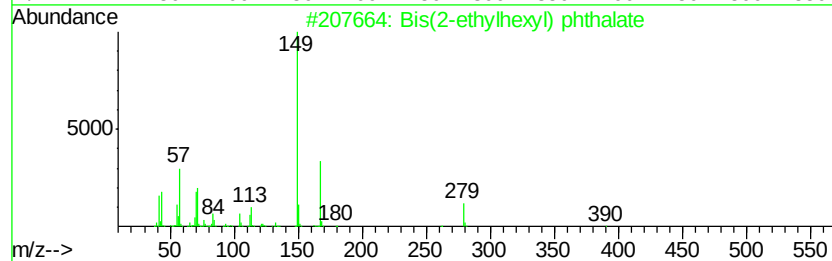
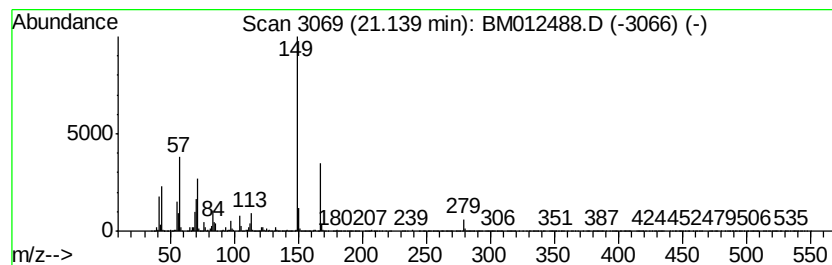
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Bis(2-ethylhexyl) phthalate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.14	18.46 ng/ul	10369100	Chrysene-d12	21.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	94
2		Phthalic acid, di(2-propylpentyl)...	390	C24H38O4	1000377-93-5	86
3		Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	86
4		Diisooctyl phthalate	390	C24H38O4	000131-20-4	81
5		Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	80



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
Data File : BM012488.D
Acq On : 27 Oct 2017 16:07
Operator : SJ/JU
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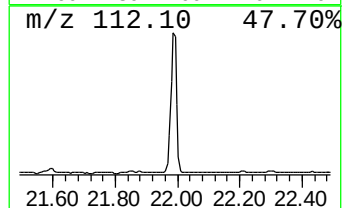
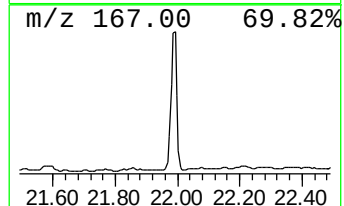
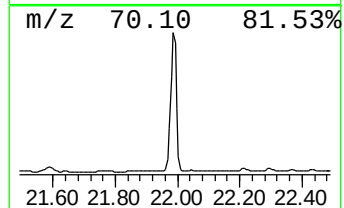
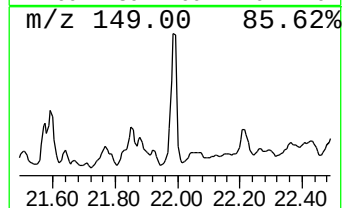
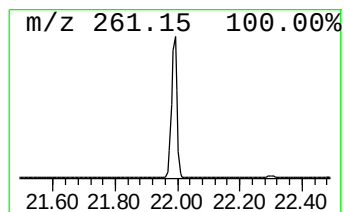
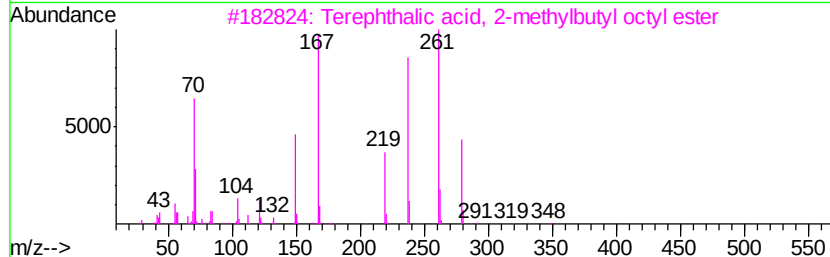
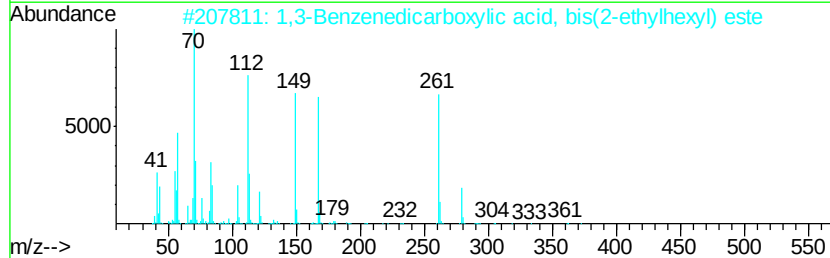
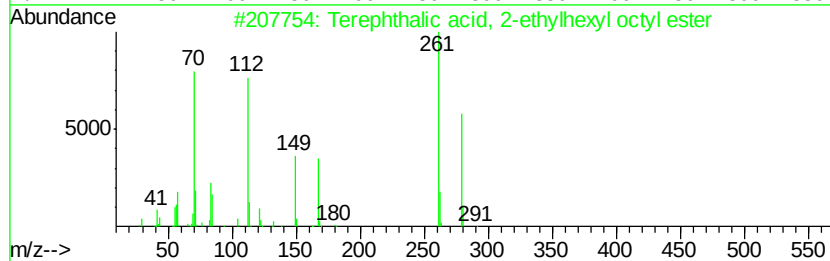
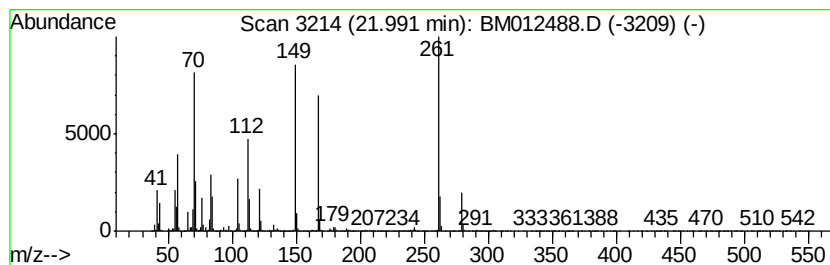
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Terephthalic acid, 2-ethylh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	75.36 ng/ul	42327900	Chrysene-d12	21.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	59
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3		Terephthalic acid, 2-methylbutyl...	348	C21H32O4	1000323-90-4	43
4		Isophthalic acid, 2-chlorophenyl...	388	C22H25ClO4	1000344-50-0	42
5		Isophthalic acid, 4-chlorophenyl...	388	C22H25ClO4	1000344-58-3	42



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
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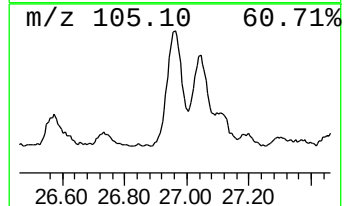
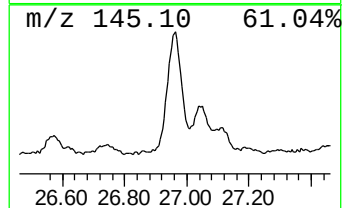
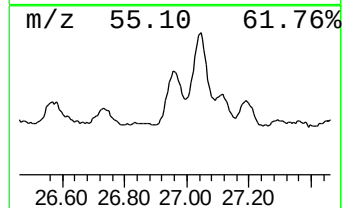
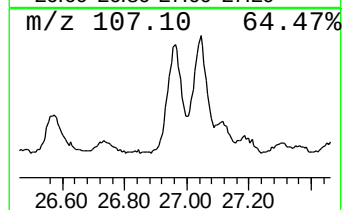
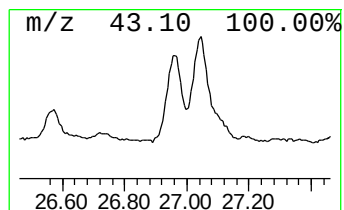
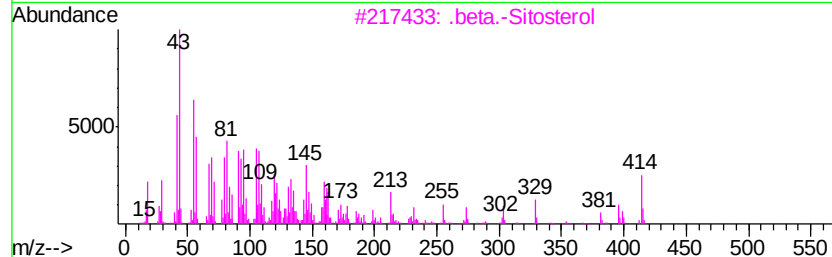
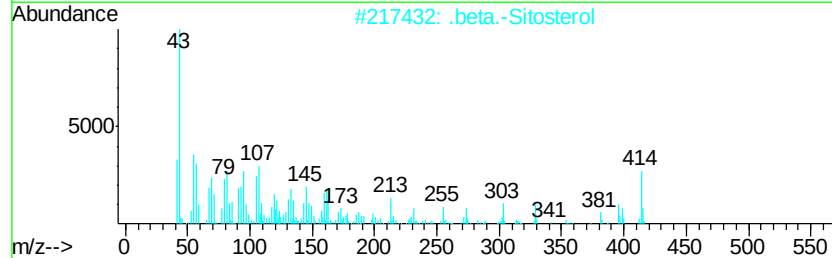
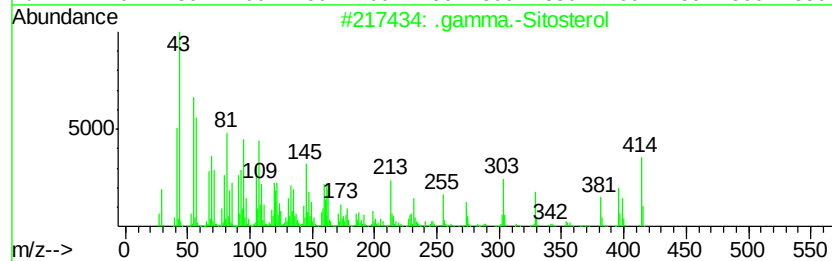
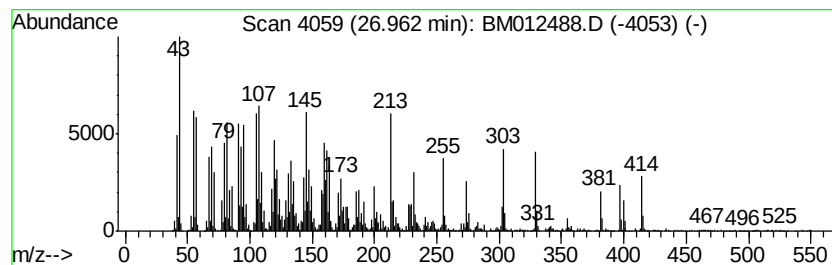
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 .gamma.-Sitosterol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.96	6.25 ng/ul	13228100	Perylene-d12	23.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 99
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 98
3		.beta.-Sitosterol	414 C29H50O	000083-46-5 38
4		5-Cholestene-3-ol, 24-methyl-	400 C28H48O	1000214-17-4 30
5		.gamma.-Sitosterol	414 C29H50O	000083-47-6 25



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
Data File : BM012488.D
Acq On : 27 Oct 2017 16:07
Operator : SJ/JU
Sample : I5873-03
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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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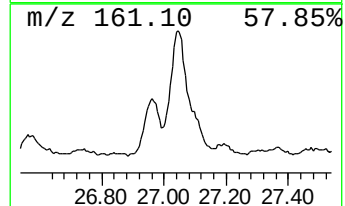
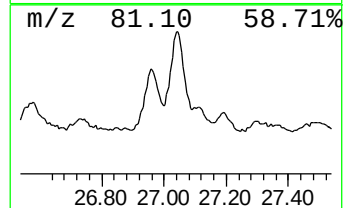
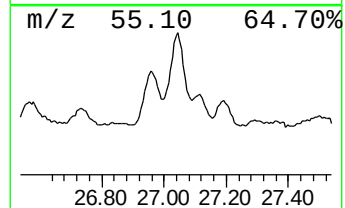
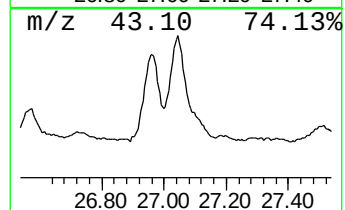
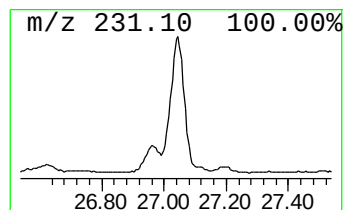
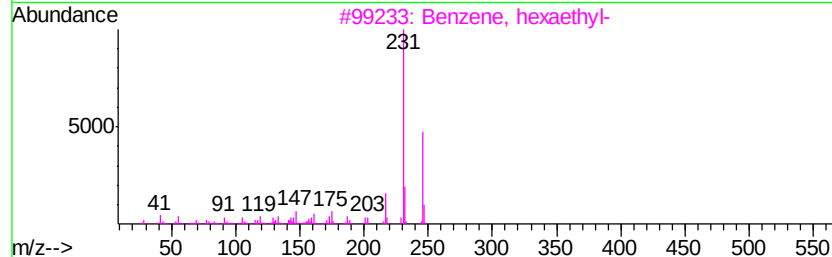
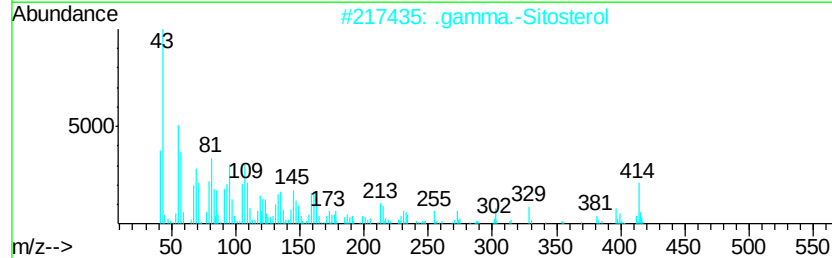
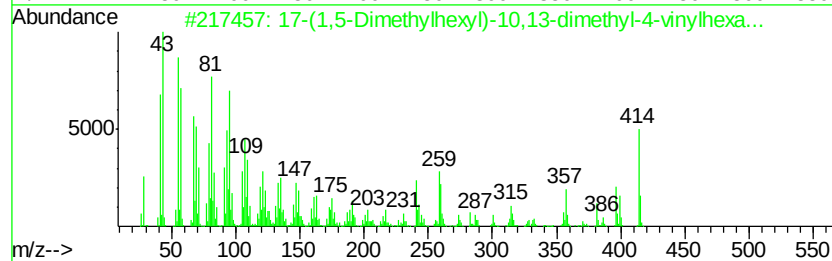
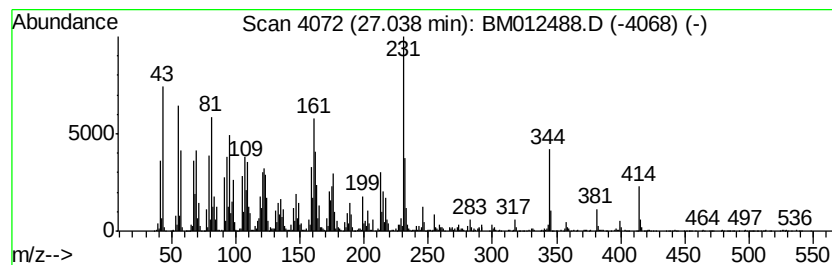
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown-03 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.04	7.84 ng/ul	16584000	Perylene-d12	23.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	43		
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	35		
3	Benzene, hexaethyl-	246	C18H30	000604-88-6	25		
4	(5-Hydroxy-3,5-dimethyl-4,5-dihy...	344	C12H13IN2O2	331868-93-0	22		
5	Quinoline, 2-[2-(3-pyridyl)ethen...	232	C16H12N2	001586-51-2	14		



Data Path : Z:\HPCHEM1\BNA_M\Data\BM102717\
 Data File : BM012488.D
 Acq On : 27 Oct 2017 16:07
 Operator : SJ/JU
 Sample : I5873-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-13(1-3)_101117

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3,5-Octadiyne	5.56	53.9	ng/ul	193713000	1	7.88	71947800	20.0
n-Decanoic acid	12.85	2.1	ng/ul	8460990	3	14.52	81496800	20.0
Dodecanoic acid	15.03	20.0	ng/ul	81496800	3	14.52	81496800	20.0
Pentadecanoic acid	17.46	17.6	ng/ul	6992730	4	17.26	7963410	20.0
cis-9-Hexadecenoic acid	18.45	25.3	ng/ul	10066000	4	17.26	7963410	20.0
Oleic Acid	19.40	248.7	ng/ul	139657000	5	21.44	11233300	20.0
Octadecanoic acid	19.53	505.9	ng/ul	284122000	5	21.44	11233300	20.0
unknown-01	20.46	40.6	ng/ul	22793500	5	21.44	11233300	20.0
unknown-02	20.56	77.5	ng/ul	43504600	5	21.44	11233300	20.0
Bis(2-ethylhexyl)...	21.14	18.5	ng/ul	10369100	5	21.44	11233300	20.0
Terephthalic acid...	21.99	75.4	ng/ul	42327900	5	21.44	11233300	20.0
.gamma.-Sitosterol	26.96	6.3	ng/ul	13228100	6	23.76	42327900	20.0
unknown-03	27.04	7.8	ng/ul	16584000	6	23.76	42327900	20.0