

Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
 Data File : BM012428.D
 Acq On : 24 Oct 2017 21:48
 Operator : SJ/JU
 Sample : I5978-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TWP-B-7

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	5.557	409	420	429	rBV	657840	941418	1.41%	0.416%
2	6.981	653	662	667	rVV	586338	1034655	1.55%	0.457%
3	7.040	667	672	680	rVB	564179	902475	1.35%	0.399%
4	7.210	696	701	709	rVB	1613023	2369010	3.55%	1.047%
5	7.416	725	736	744	rVB	1884071	3120663	4.68%	1.379%
6	7.881	805	815	821	rBV	1940274	3161323	4.74%	1.397%
7	8.022	833	839	846	rVB	1722435	2635281	3.95%	1.165%
8	8.581	927	934	945	rBV	1532225	2656302	3.98%	1.174%
9	9.034	1004	1011	1019	rVB	2099435	3366051	5.05%	1.488%
10	9.122	1019	1026	1035	rVB	398088	736788	1.10%	0.326%
11	9.757	1085	1134	1136	rBV3	9280208	66683588	100.00%	29.477%
12	10.051	1176	1184	1189	rBV	15369161	25446623	38.16%	11.249%
13	10.098	1189	1192	1198	rVV3	2887915	4906695	7.36%	2.169%
14	10.222	1205	1213	1219	rVB3	684225	1537009	2.30%	0.679%
15	10.292	1219	1225	1236	rBV2	3522375	6135163	9.20%	2.712%
16	10.675	1282	1290	1296	rBV	2369107	3980989	5.97%	1.760%
17	11.410	1409	1415	1422	rBV	942401	1615182	2.42%	0.714%
18	13.228	1719	1724	1730	rBV	508151	711386	1.07%	0.314%
19	13.916	1831	1841	1847	rBV	5077857	6983466	10.47%	3.087%
20	14.198	1885	1889	1899	rVB	5518410	8181337	12.27%	3.617%
21	14.510	1932	1942	1948	rBV2	4165838	6311564	9.46%	2.790%
22	14.692	1967	1973	1977	rBV	470497	711279	1.07%	0.314%
23	15.498	2104	2110	2116	rBV	7117805	9949281	14.92%	4.398%
24	15.604	2123	2128	2138	rBV	1589427	2291058	3.44%	1.013%
25	16.398	2259	2263	2269	rVV2	384895	713486	1.07%	0.315%
26	16.727	2314	2319	2328	rBV2	403757	901185	1.35%	0.398%
27	17.245	2401	2407	2412	rBV2	4635624	6663632	9.99%	2.946%
28	17.345	2418	2424	2434	rVB	7757332	10619044	15.92%	4.694%
29	18.168	2561	2564	2569	rVV	871280	1090926	1.64%	0.482%
30	19.633	2807	2813	2827	rVB	9102114	12022010	18.03%	5.314%
31	19.780	2833	2838	2843	rBV	1356420	1640055	2.46%	0.725%
32	21.415	3111	3116	3121	rBV	6149756	7533153	11.30%	3.330%
33	23.574	3476	3483	3490	rBV2	6074441	11499826	17.25%	5.083%
34	23.715	3501	3507	3515	rVB2	3591748	7169700	10.75%	3.169%

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ClientSampleId :
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 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

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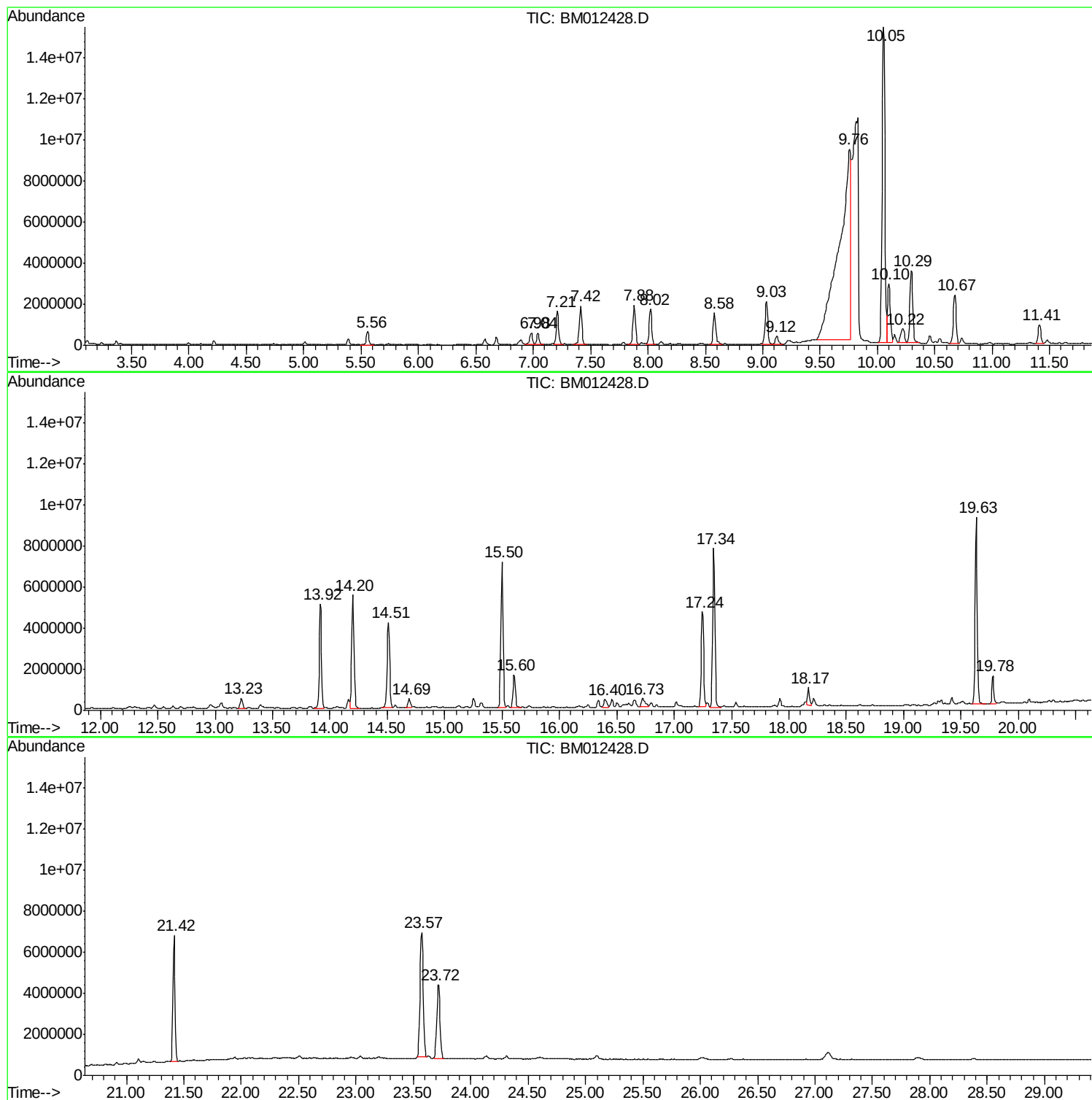
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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



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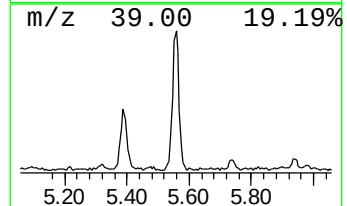
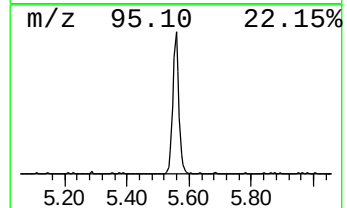
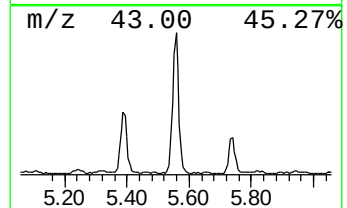
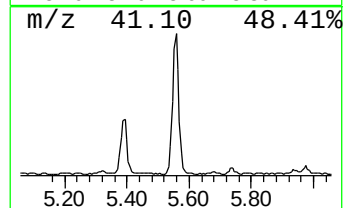
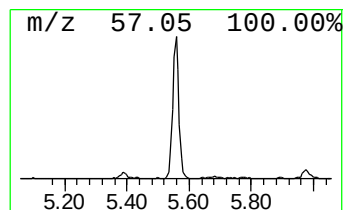
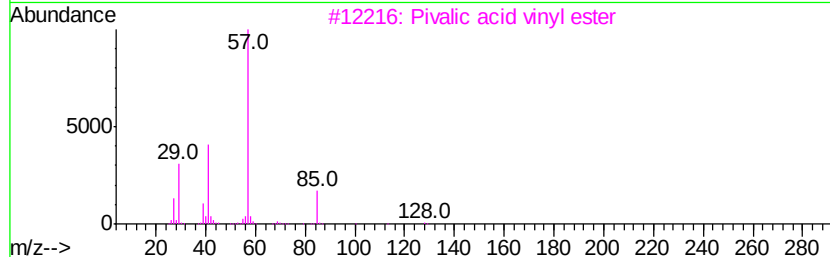
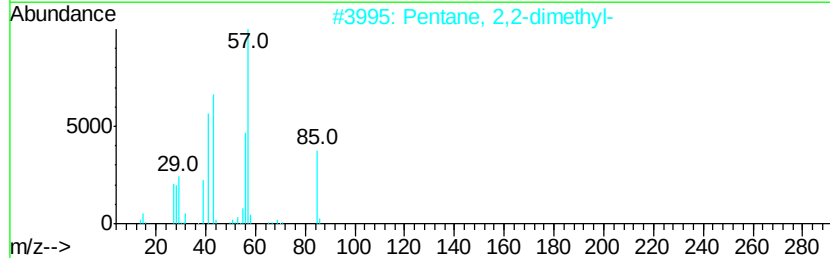
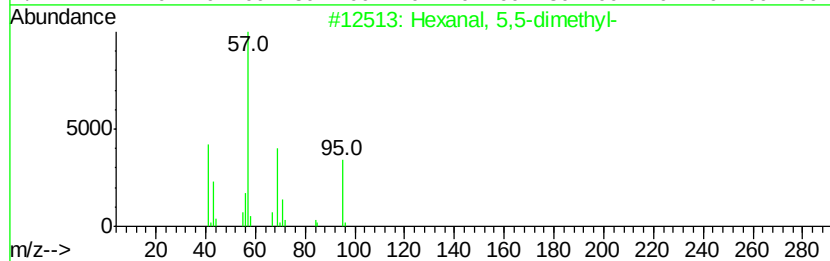
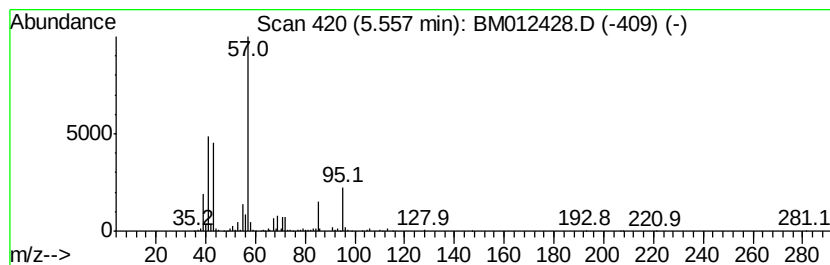
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	5.96 ng/ul	941418	1,4-Dichlorobenzene-d4	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal, 5,5-dimethyl-	128	C8H16O	055320-58-6	42
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	35
3		Pivalic acid vinyl ester	128	C7H12O2	003377-92-2	35
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	25
5		Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	23



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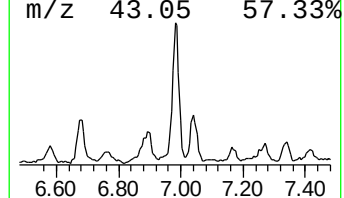
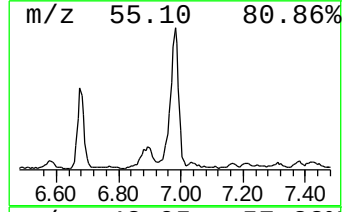
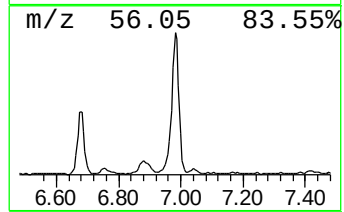
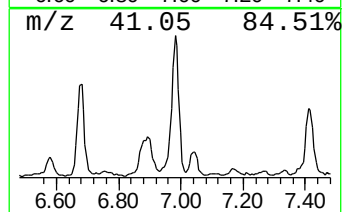
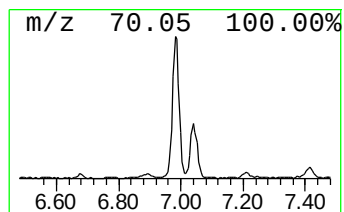
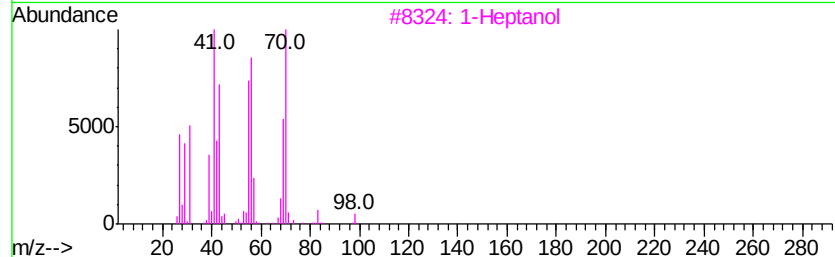
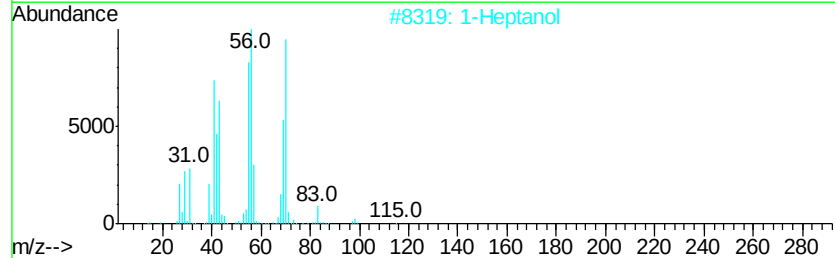
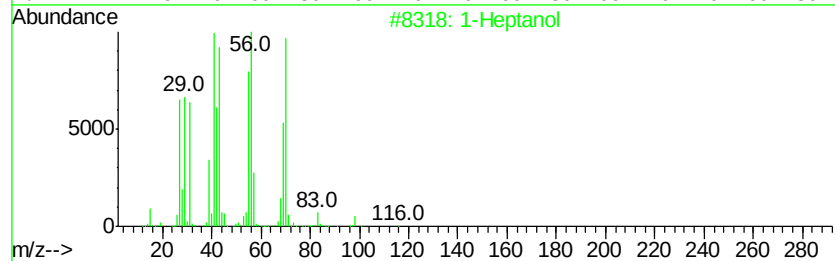
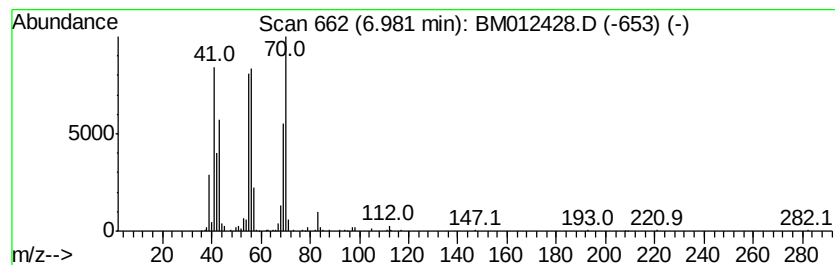
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	6.55 ng/ul	1034660	1,4-Dichlorobenzene-d4	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptanol	116	C7H16O	000111-70-6	83
2		1-Heptanol	116	C7H16O	000111-70-6	83
3		1-Heptanol	116	C7H16O	000111-70-6	83
4		1-Heptanol	116	C7H16O	000111-70-6	78
5		Formic acid, heptyl ester	144	C8H16O2	000112-23-2	78



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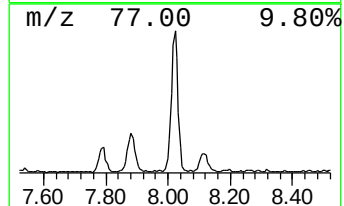
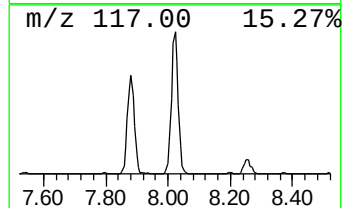
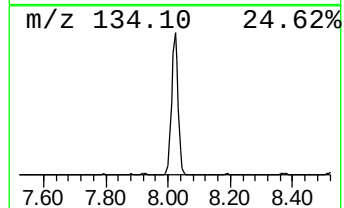
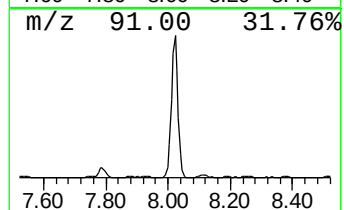
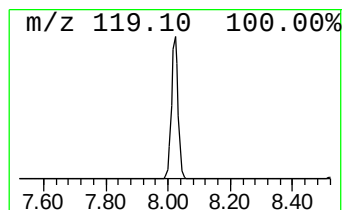
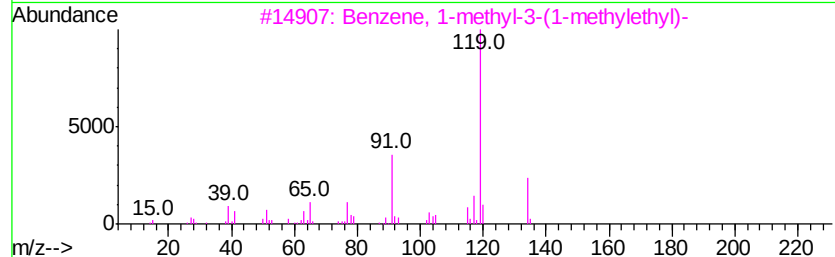
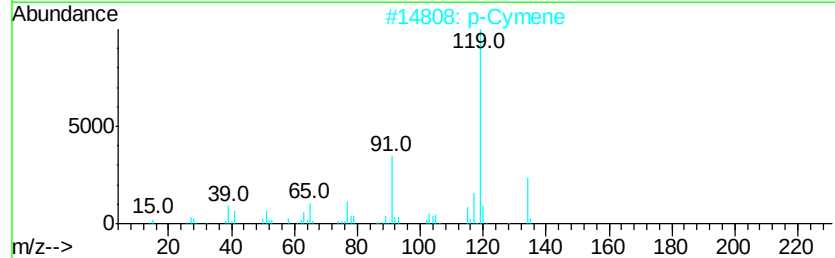
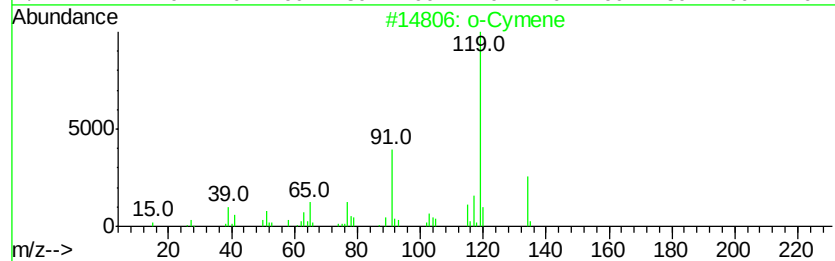
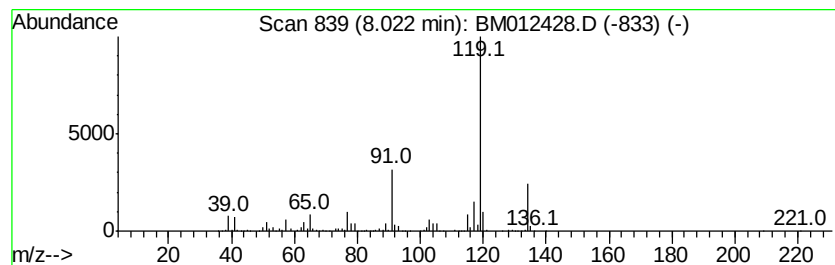
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	16.67 ng/ul	2635280	1,4-Dichlorobenzene-d4	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	97
2		p-Cymene	134	C10H14	000099-87-6	96
3		Benzene, 1-methyl-3-(1-methylethyl-...	134	C10H14	000535-77-3	96
4		o-Cymene	134	C10H14	000527-84-4	94
5		o-Cymene	134	C10H14	000527-84-4	93



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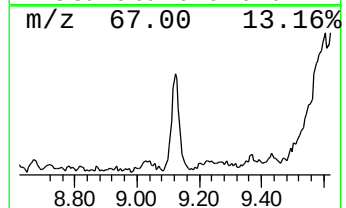
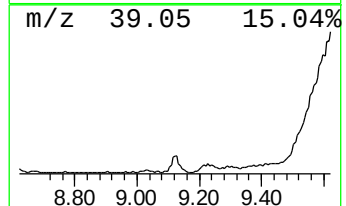
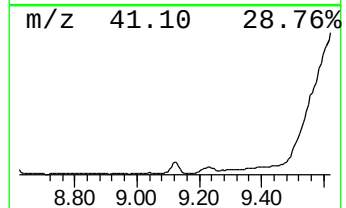
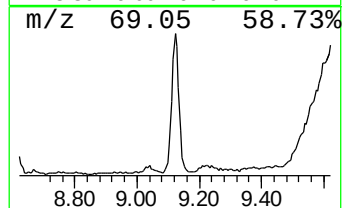
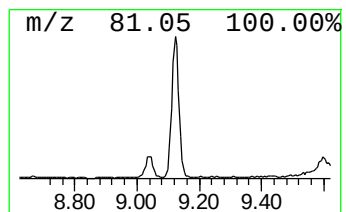
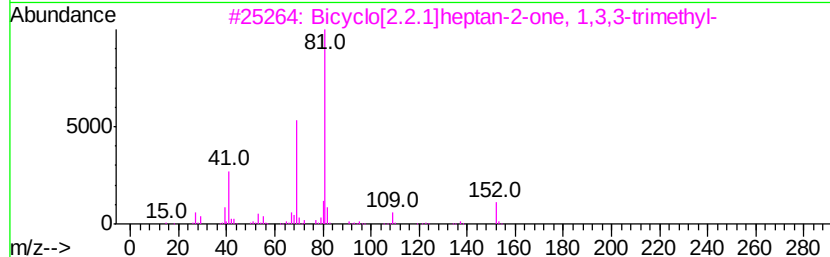
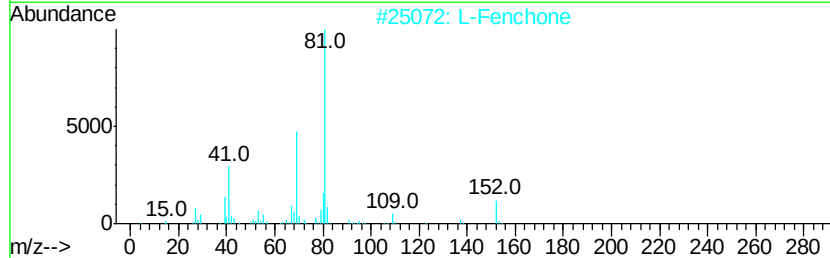
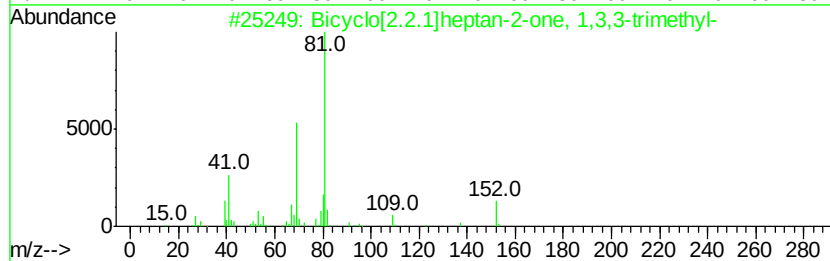
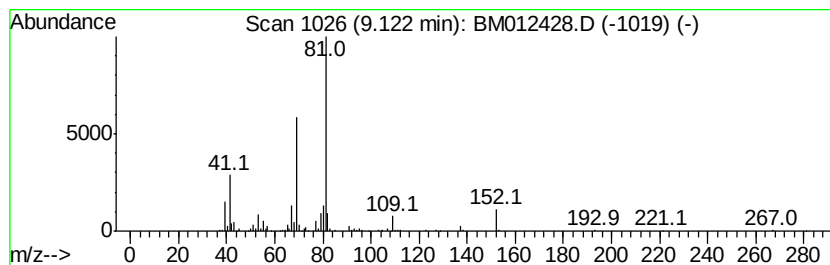
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Bicyclo[2.2.1]heptan-2-one, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	4.66 ng/ul	736788	1,4-Dichlorobenzene-d4	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	91
2		L-Fenchone	152	C10H16O	007787-20-4	91
3		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	90
4		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	80
5		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	80



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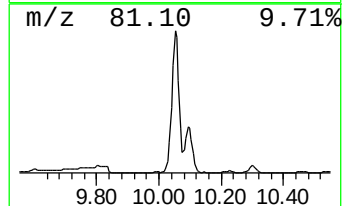
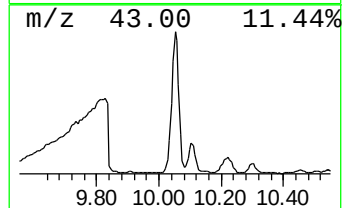
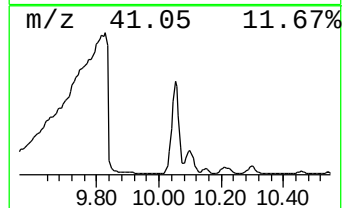
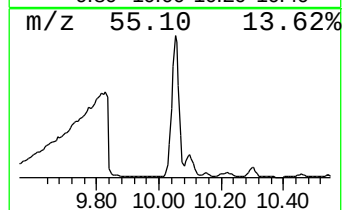
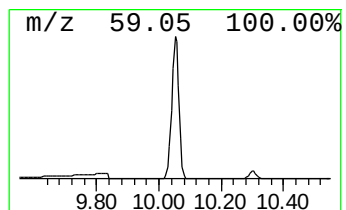
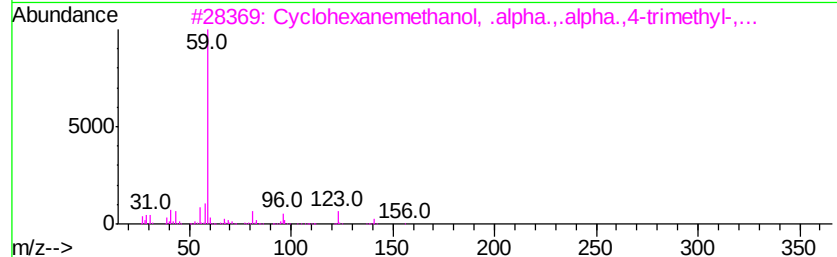
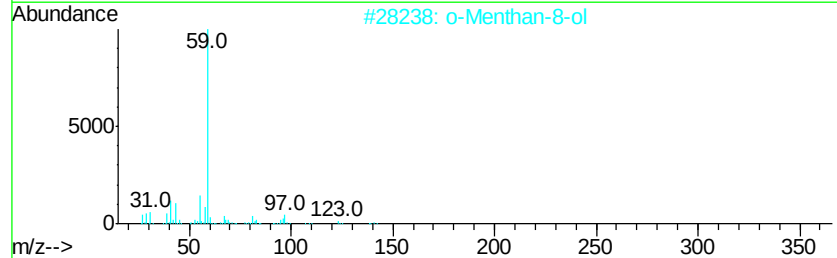
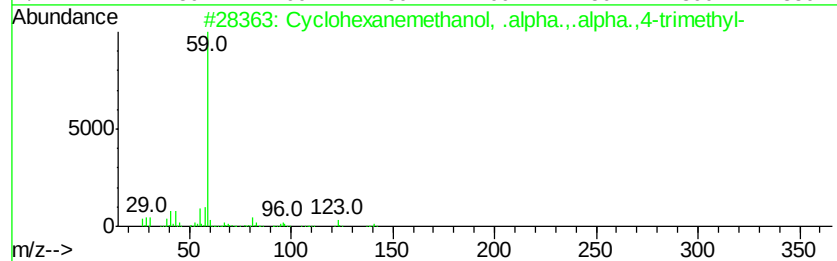
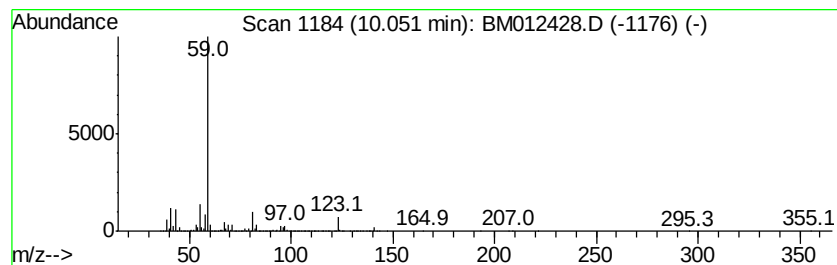
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexanemethanol, .alpha... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	127.84 ng/ul	25446600	Napthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanemethanol, .alpha...al...	156	C10H20O	000498-81-7	83
2		o-Menthan-8-ol	156	C10H20O	343855-44-7	78
3		Cyclohexanemethanol, .alpha...al...	156	C10H20O	005114-00-1	78
4		Cyclohexanemethanol, .alpha...al...	156	C10H20O	000498-81-7	78
5		Cyclohexanemethanol, .alpha...al...	156	C10H20O	007322-63-6	64



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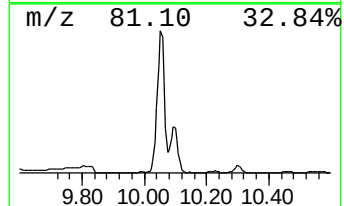
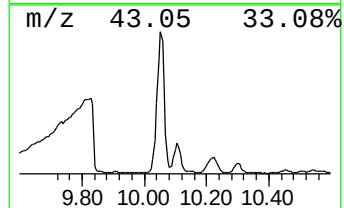
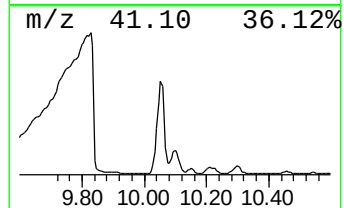
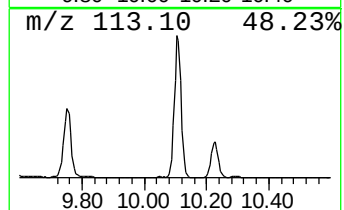
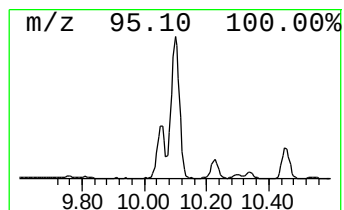
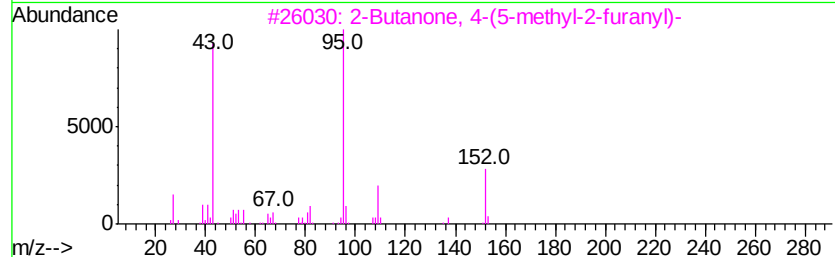
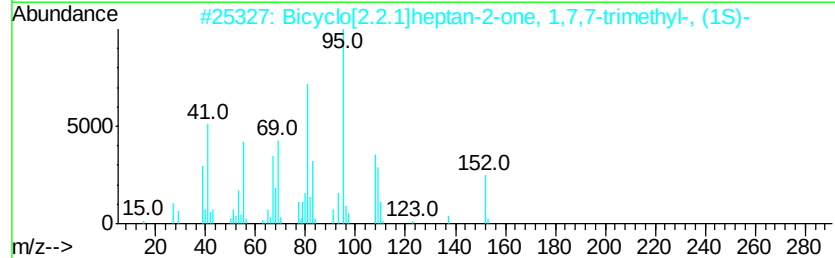
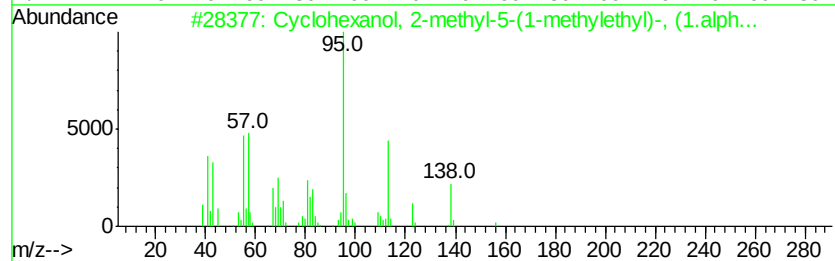
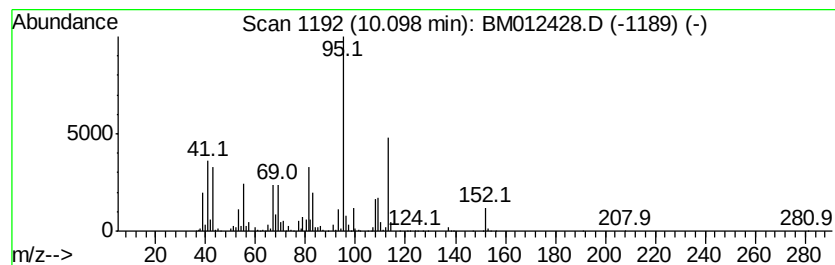
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Cyclohexanol, 2-methyl-5-(1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	24.65 ng/ul	4906700	Naphthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 2-methyl-5-(1-meth...	156	C10H20O	000499-69-4	72
2		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	38
3		2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	38
4		(+)-2-Bornanone	152	C10H16O	000464-49-3	38
5		6-Methyl-2-heptyne	110	C8H14	051065-64-6	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
Data File : BM012428.D
Acq On : 24 Oct 2017 21:48
Operator : SJ/JU
Sample : I5978-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TWP-B-7

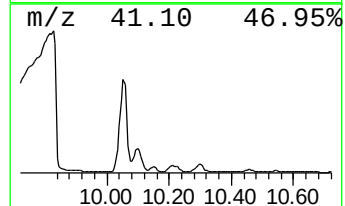
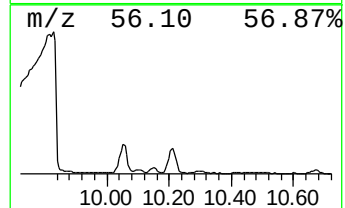
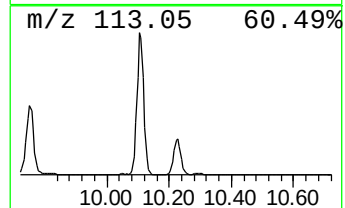
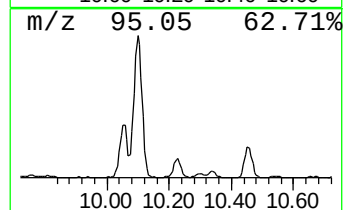
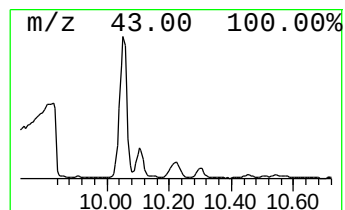
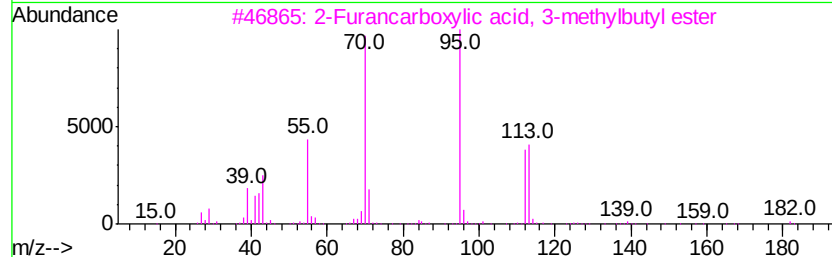
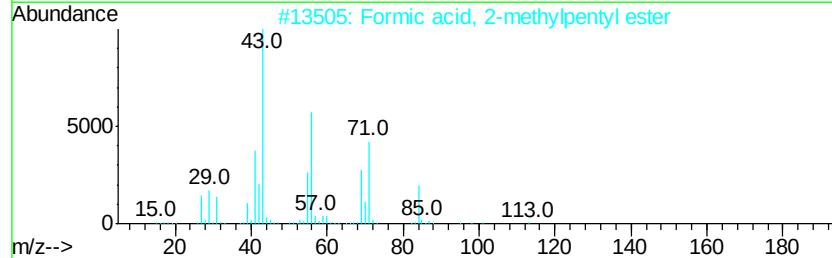
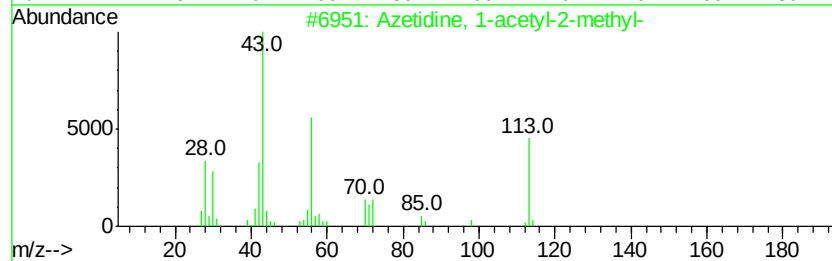
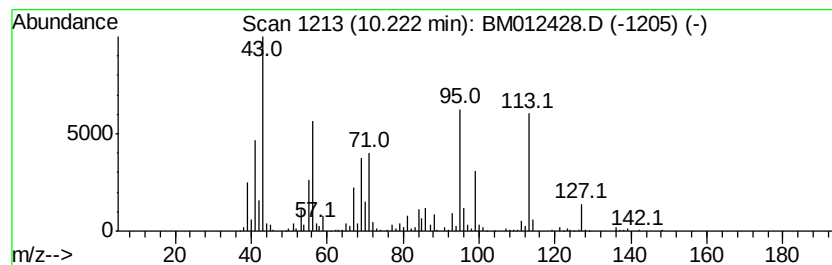
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	7.72 ng/ul	1537010	Naphthalene-d8	10.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Azetidine, 1-acetyl-2-methyl-	113	C6H11NO	050837-77-9	27
2		Formic acid, 2-methylpentyl ester	130	C7H14O2	381670-34-4	27
3		2-Furancarboxylic acid, 3-methyl...	182	C10H14O3	000615-12-3	27
4		Caprolactam	113	C6H11NO	000105-60-2	22
5		Caprolactam	113	C6H11NO	000105-60-2	22



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
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Acq On : 24 Oct 2017 21:48
Operator : SJ/JU
Sample : I5978-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TWP-B-7

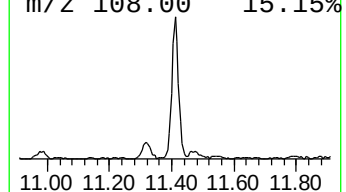
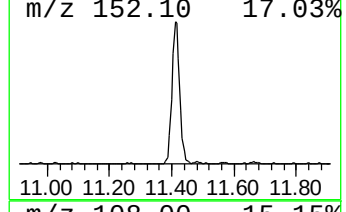
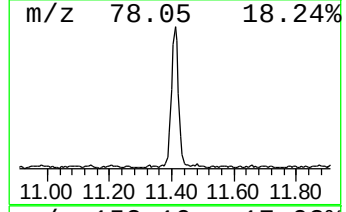
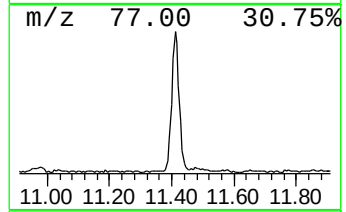
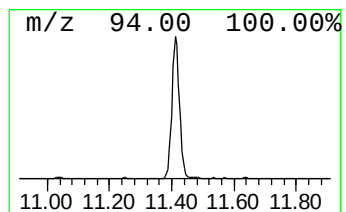
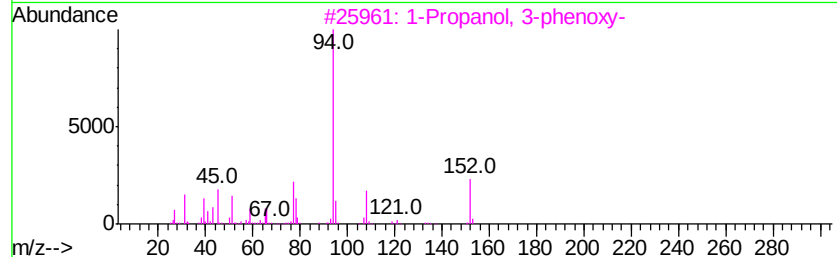
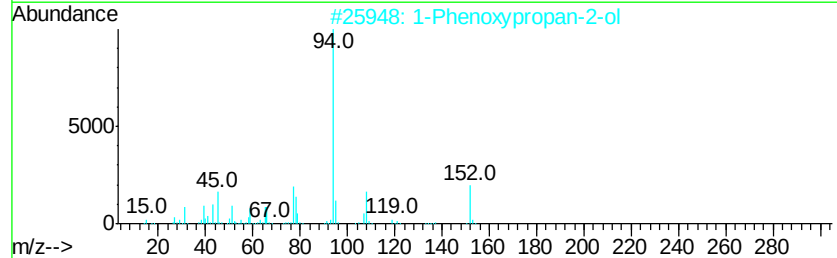
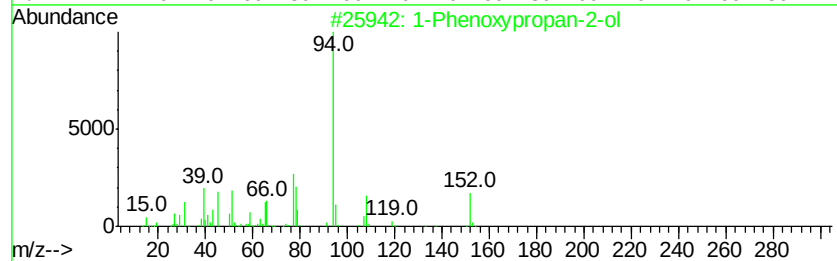
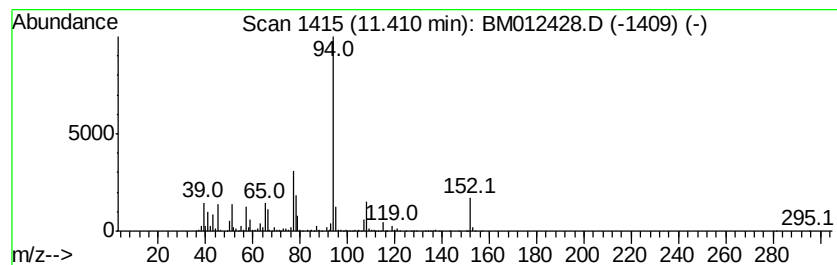
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	8.11 ng/ul	1615180	Napthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
3		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
4		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5		3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
Data File : BM012428.D
Acq On : 24 Oct 2017 21:48
Operator : SJ/JU
Sample : I5978-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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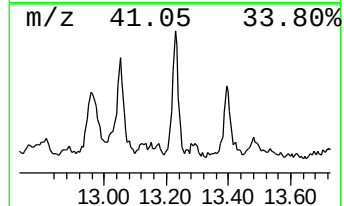
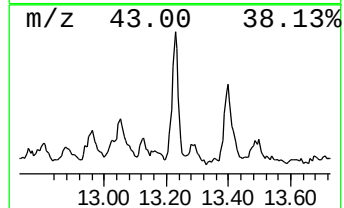
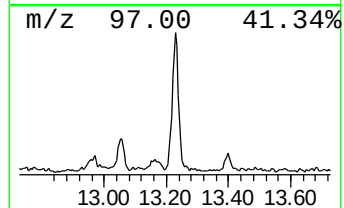
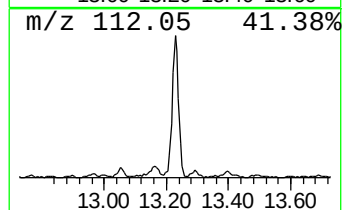
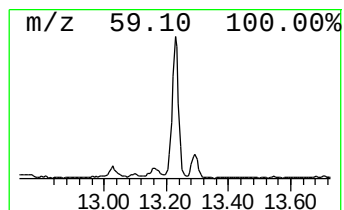
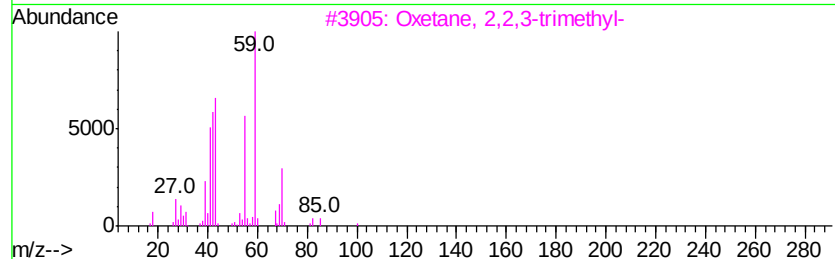
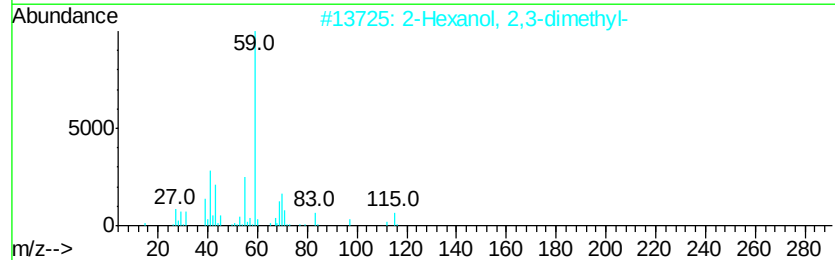
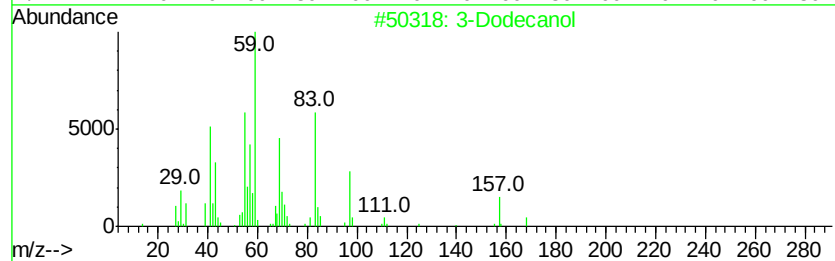
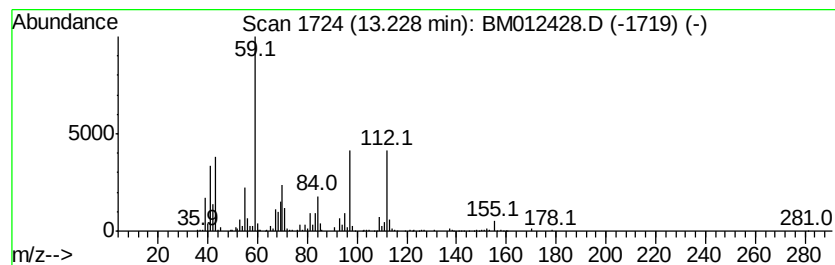
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	2.25 ng/ul	711386	Acenaphthene-d10	14.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Dodecanol	186	C12H26O	010203-30-2	42
2		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	38
3		Oxetane, 2,2,3-trimethyl-	100	C6H12O	023120-43-6	25
4		Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	25
5		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	25



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
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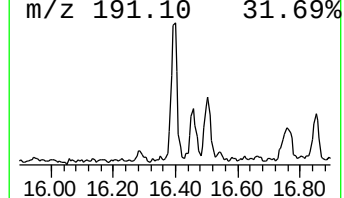
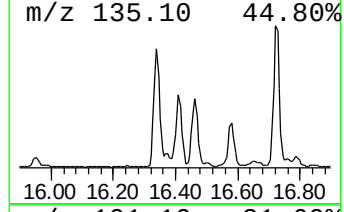
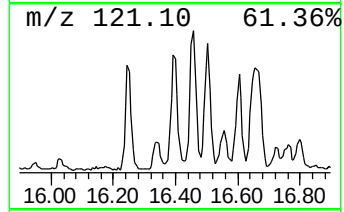
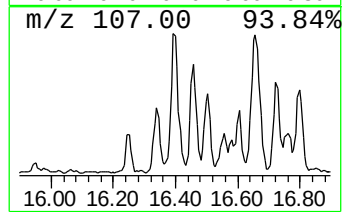
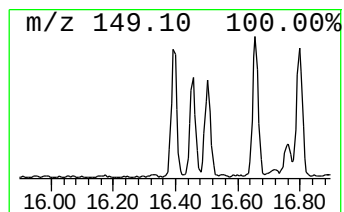
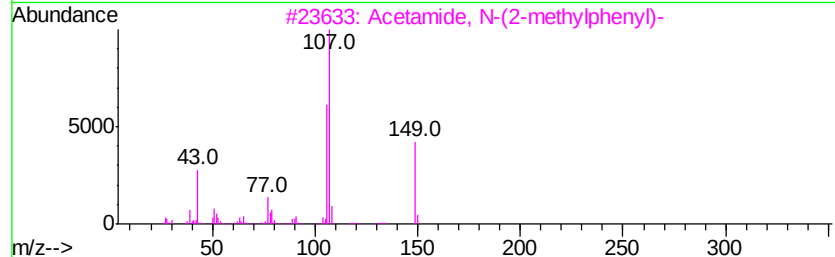
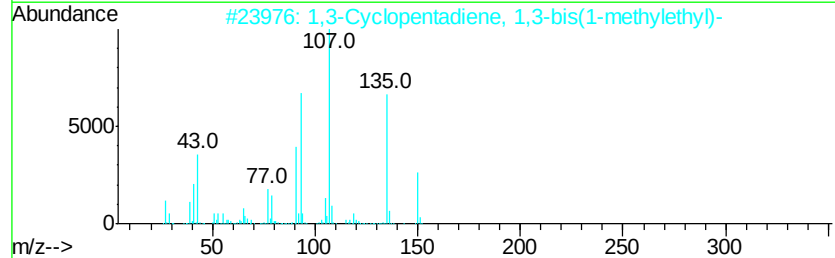
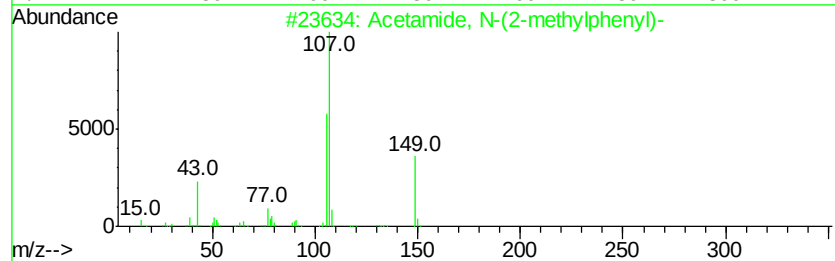
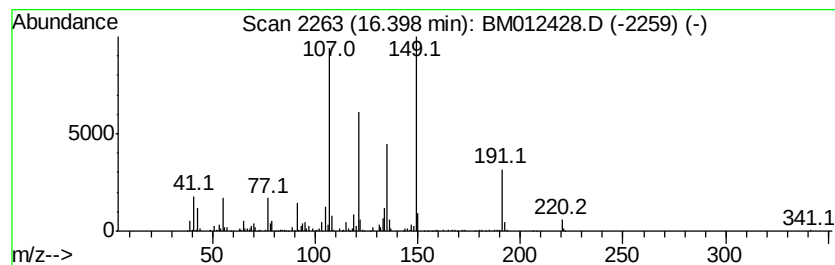
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

Peak Number 10 Acetamide, N-(2-methylphenyl)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.14 ng/ul	713486	Phenanthrene-d10	17.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Acetamide, N-(2-methylphenyl)-	149 C9H11NO	000120-66-1	50
2	1,3-Cyclopentadiene, 1,3-bis(1-m...	150 C11H18	123278-27-3	45
3	Acetamide, N-(2-methylphenyl)-	149 C9H11NO	000120-66-1	43
4	Acetamide, N-(3-methylphenyl)-	149 C9H11NO	000537-92-8	38
5	Pyridine-3-carbonitrile, 1,2-dih...	191 C9H9N3O2	220098-92-0	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
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Sample : I5978-01
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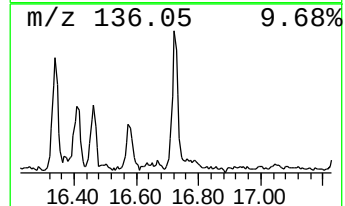
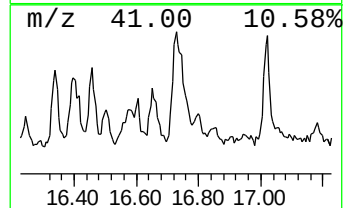
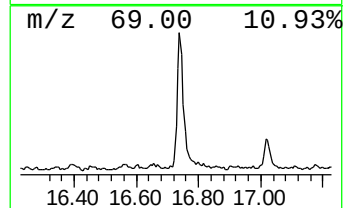
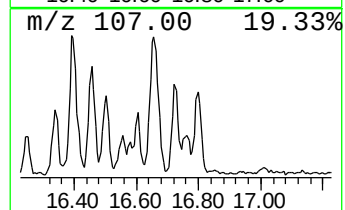
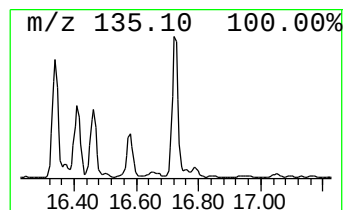
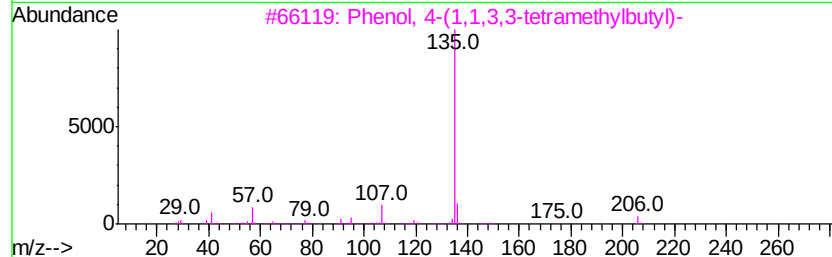
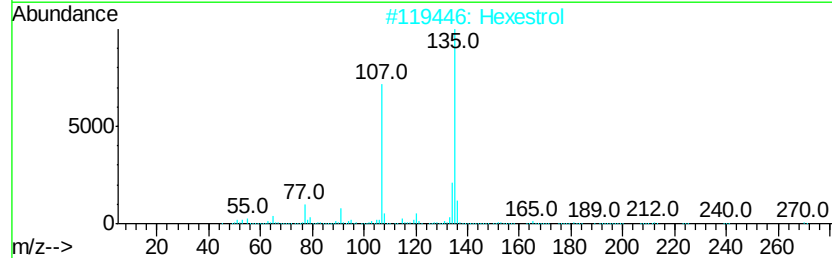
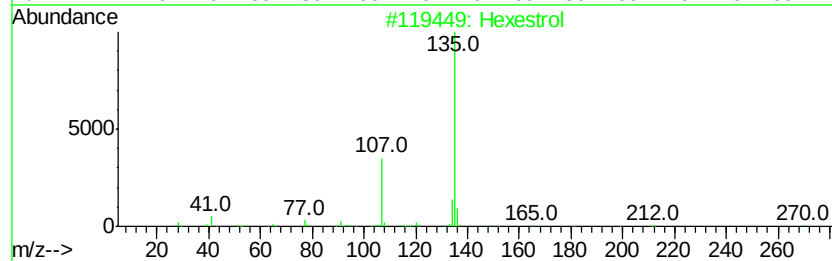
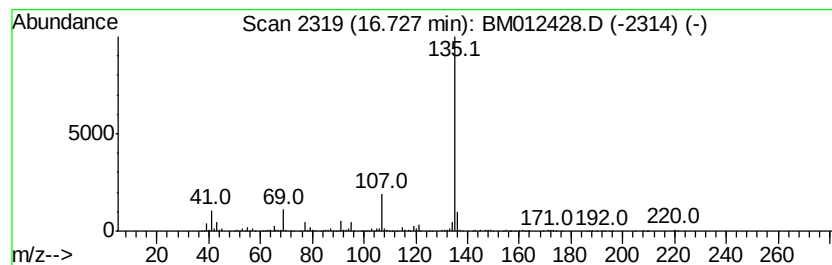
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 Hexestrol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.70 ng/ul	901185	Phenanthrene-d10	17.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexestrol		270 C18H22O2	000084-16-2 64
2	Hexestrol		270 C18H22O2	000084-16-2 59
3	Phenol, 4-(1,1,3,3-tetramethylbu...		206 C14H22O	000140-66-9 59
4	Carbamic acid, N-[1,1-bis(triflu...		413 C19H25F6N02	296242-69-8 59
5	4-(1,1-Dimethylpropyl)phenyl ace...		206 C13H18O2	1000373-45-3 59



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102417\
Data File : BM012428.D
Acq On : 24 Oct 2017 21:48
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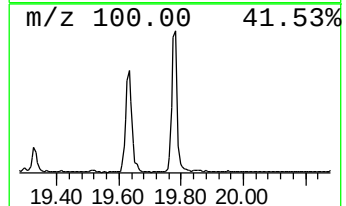
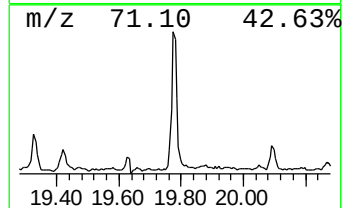
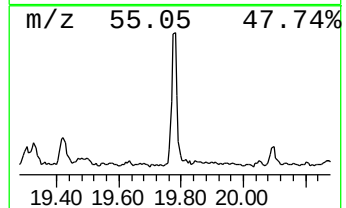
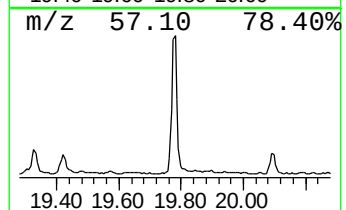
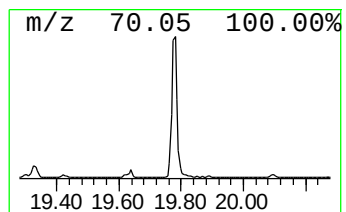
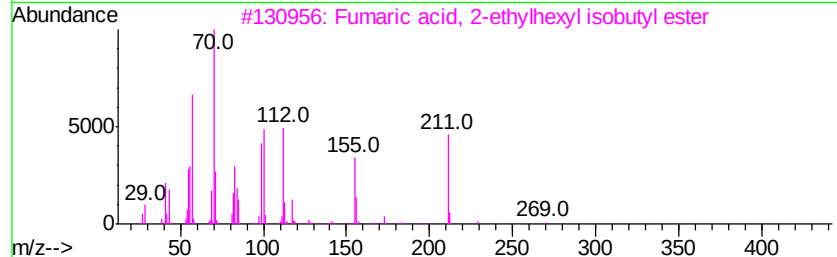
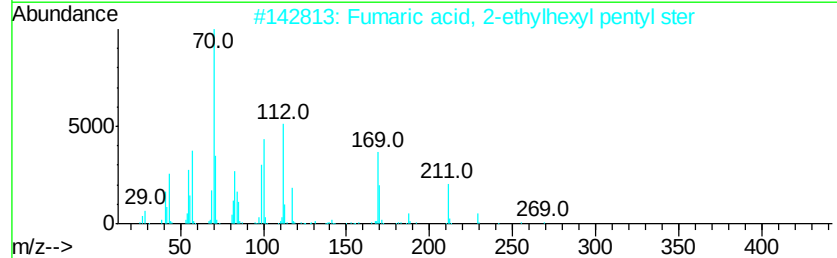
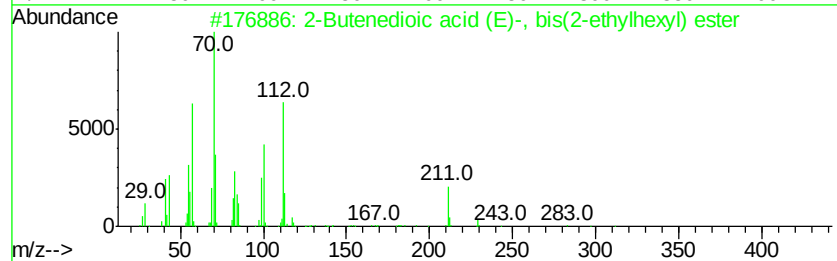
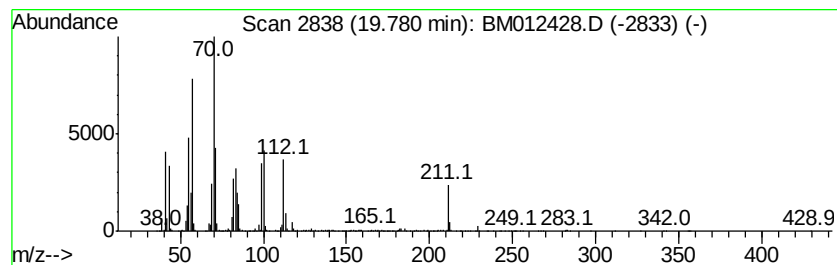
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 2-Butenedioic acid (E)-, bi... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	4.35 ng/ul	1640060	Chrysene-d12	21.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	80
2		Fumaric acid, 2-ethylhexyl penty...	298	C17H30O4	1000339-13-9	78
3		Fumaric acid, 2-ethylhexyl isobu...	284	C16H28O4	1000339-13-7	47
4		Propanoic acid, 2,2-dimethyl-, 2...	214	C13H26O2	016387-18-1	43
5		Carbonic acid, butyl 2-ethylhexy...	230	C13H26O3	1000357-84-4	43



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM102417\
Data File : BM012428.D
Acq On : 24 Oct 2017 21:48
Operator : SJ/JU
Sample : I5978-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TWP-B-7

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
unknown-01	5.56	6.0	ng/ul	941418	1	7.88	3161320	20.0
1-Heptanol	6.98	6.5	ng/ul	1034660	1	7.88	3161320	20.0
o-Cymene	8.02	16.7	ng/ul	2635280	1	7.88	3161320	20.0
Bicyclo[2.2.1]hep...	9.12	4.7	ng/ul	736788	1	7.88	3161320	20.0
Cyclohexanemethan...	10.05	127.8	ng/ul	25446600	2	10.67	3980990	20.0
Cyclohexanol, 2-m...	10.10	24.6	ng/ul	4906700	2	10.67	3980990	20.0
unknown-02	10.22	7.7	ng/ul	1537010	2	10.67	3980990	20.0
1-Phenoxypropan-2-ol	11.41	8.1	ng/ul	1615180	2	10.67	3980990	20.0
unknown-03	13.23	2.3	ng/ul	711386	3	14.51	6311560	20.0
Acetamide, N-(2-m...	16.40	2.1	ng/ul	713486	4	17.24	6663630	20.0
Hexestrol	16.73	2.7	ng/ul	901185	4	17.24	6663630	20.0
2-Butenedioic aci...	19.78	4.3	ng/ul	1640060	5	21.42	7533150	20.0