

Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
 Data File : BN000836.D
 Acq On : 23 Apr 2018 20:26
 Operator : JU/SJ
 Sample : J2467-15
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 A3Y06

Integration Parameters: events.e
 Integrator: ChemStation
 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_N\METHODS\SOM-EPA-BN041918-PAH.M
 Title : ??? S

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.711	455	463	468	rBV	59154	91091	2.86%	0.259%
2	6.799	641	648	659	rVB	191042	295406	9.27%	0.840%
3	6.969	670	677	688	rBV	682002	997867	31.31%	2.837%
4	7.158	703	709	720	rVB	662192	1003227	31.48%	2.852%
5	7.622	781	788	794	rBV	601922	902224	28.31%	2.565%
6	7.693	794	800	808	rVB	201362	287849	9.03%	0.818%
7	8.322	900	907	919	rVB	562182	854632	26.82%	2.429%
8	8.705	967	972	976	rBV	61628	92886	2.91%	0.264%
9	8.763	976	982	988	rVV	734603	1139544	35.76%	3.239%
10	9.481	1097	1104	1111	rBV	588081	941421	29.54%	2.676%
11	10.010	1187	1194	1204	rBV	902410	1420367	44.57%	4.037%
12	10.387	1251	1258	1265	rBV	849094	1358279	42.62%	3.861%
13	11.675	1471	1477	1486	rBV	64265	99878	3.13%	0.284%
14	12.863	1673	1679	1685	rVB	31121	44150	1.39%	0.125%
15	13.163	1725	1730	1736	rBV	54266	76724	2.41%	0.218%
16	13.669	1810	1816	1829	rVB	1547350	2075544	65.13%	5.900%
17	13.940	1855	1862	1872	rBV	1794313	2648504	83.11%	7.529%
18	14.251	1908	1915	1924	rBV2	1141844	1689971	53.03%	4.804%
19	14.451	1944	1949	1957	rBV	113286	163343	5.13%	0.464%
20	14.939	2026	2032	2039	rVB	28626	39996	1.26%	0.114%
21	15.251	2078	2085	2094	rBV	2184397	3060507	96.03%	8.700%
22	15.363	2099	2104	2114	rBV	674285	893142	28.03%	2.539%
23	16.998	2376	2382	2392	rVB	1343854	1840678	57.76%	5.232%
24	17.098	2392	2399	2412	rBV	2236815	3094429	97.10%	8.796%
25	17.681	2494	2498	2505	rBV2	315746	391166	12.27%	1.112%
26	19.398	2784	2790	2796	rBV2	2336357	3186887	100.00%	9.059%
27	21.198	3091	3096	3103	rBV	1324297	1641692	51.51%	4.667%
28	22.257	3271	3276	3288	rBV2	225130	367822	11.54%	1.046%
29	22.763	3358	3362	3367	rVB	53076	71088	2.23%	0.202%
30	23.251	3438	3445	3452	rBV2	1468111	2555757	80.20%	7.265%
31	23.316	3452	3456	3460	rVV	73838	114278	3.59%	0.325%
32	23.386	3461	3468	3479	rVB	858697	1504814	47.22%	4.278%
33	23.939	3558	3562	3571	rVB	64587	116434	3.65%	0.331%
34	24.663	3680	3685	3691	rVB2	63361	117916	3.70%	0.335%

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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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Title : ??? S

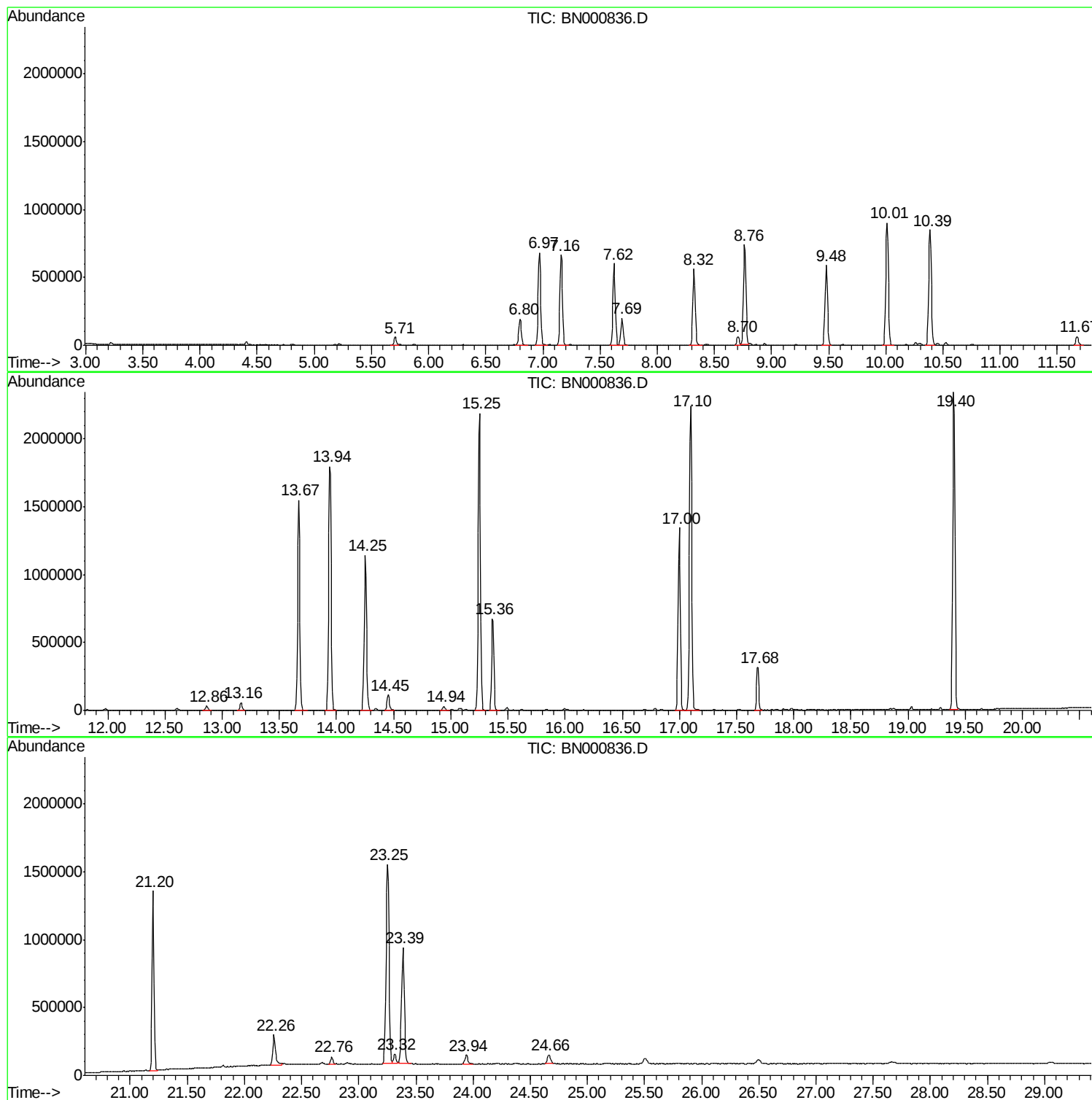
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Quant Method : Z:\HPCHEM1\BNA N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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



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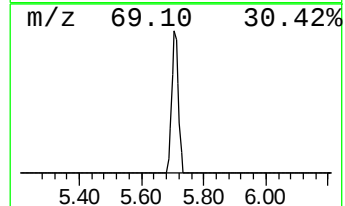
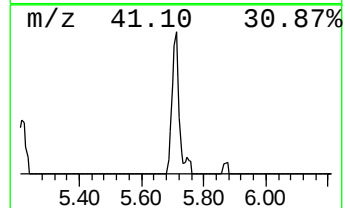
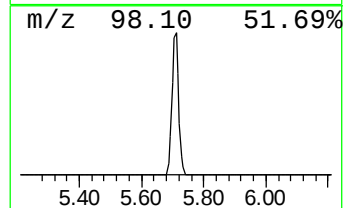
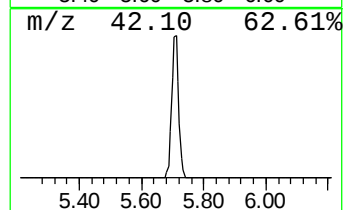
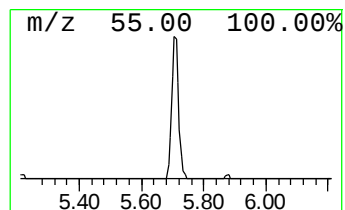
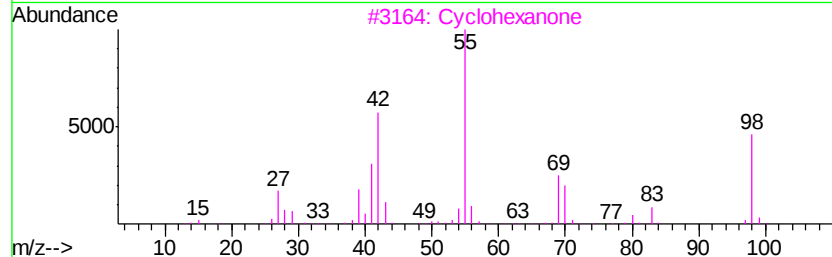
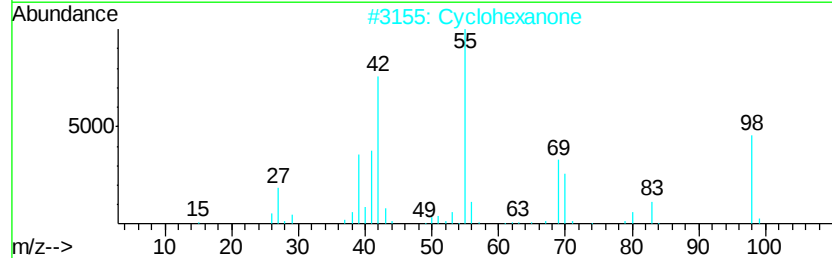
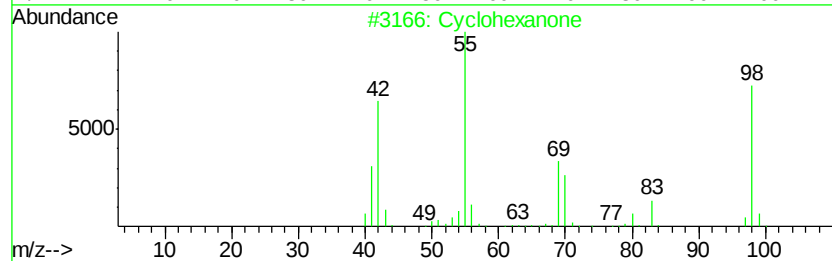
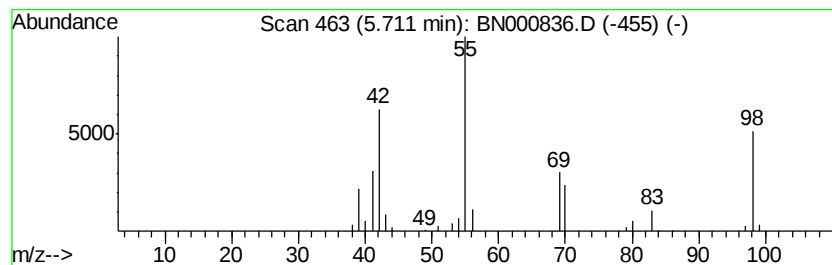
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cyclohexanone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	2.02 ng/ul	91091	1,4-Dichlorobenzene-d4	7.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	94
2			Cyclohexanone	98	C6H10O	000108-94-1	91
3			Cyclohexanone	98	C6H10O	000108-94-1	91
4			Cyclohexanone	98	C6H10O	000108-94-1	91
5			Cyclohexanone	98	C6H10O	000108-94-1	83



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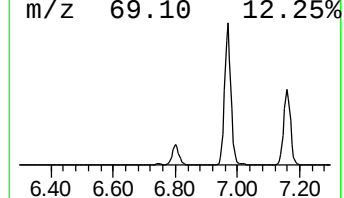
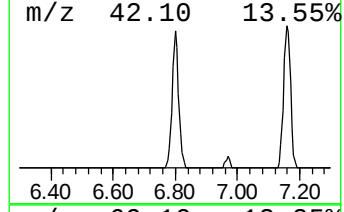
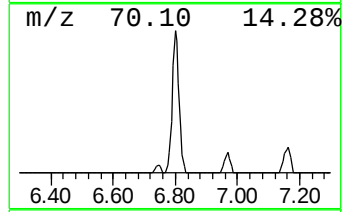
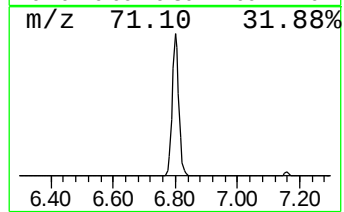
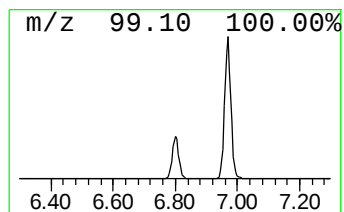
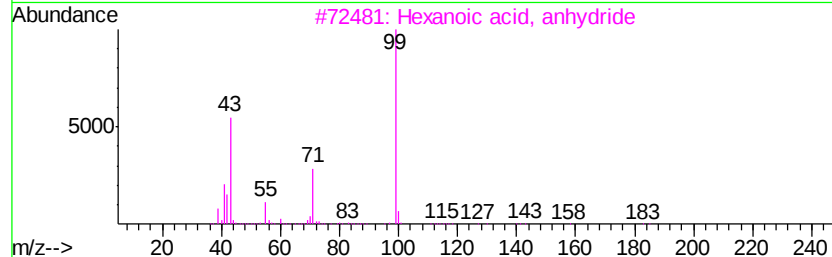
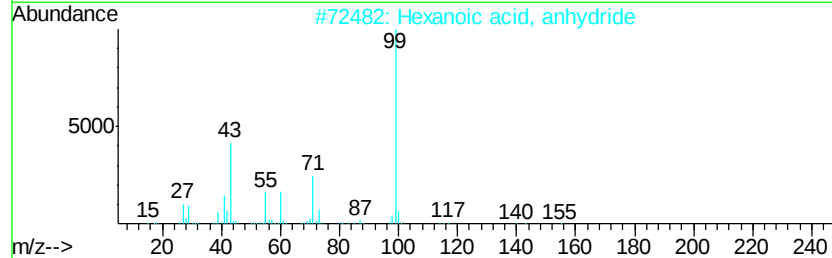
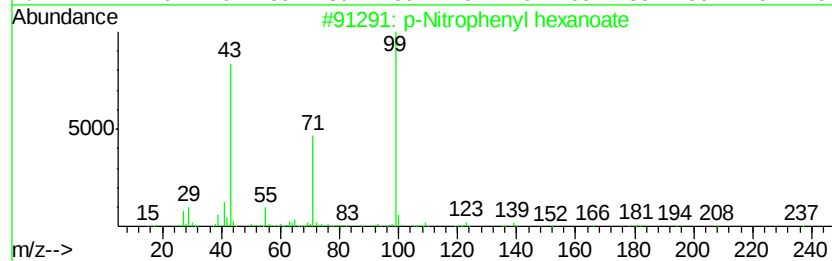
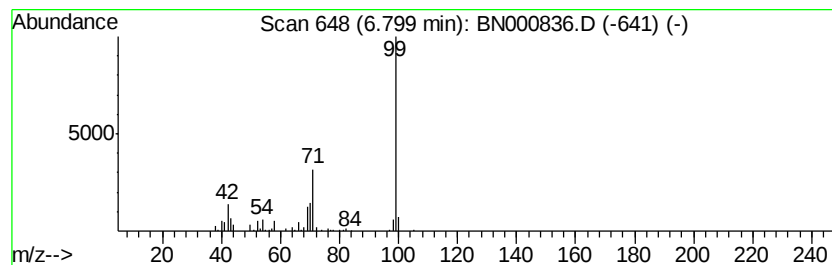
Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 p-Nitrophenyl hexanoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.80	6.55 ng/ul	295406	1,4-Dichlorobenzene-d4	7.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Nitrophenyl hexanoate	237	C12H15N04	000956-75-2	53
2	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50
3	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50
4	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50
5	2-Thioxo-dihydropyrimidine-4,6-d...	359	C17H21N5O2S	1000304-28-6	50



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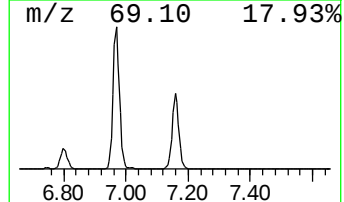
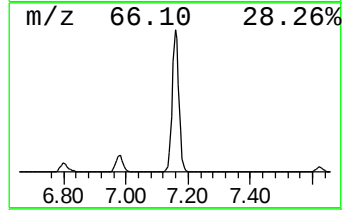
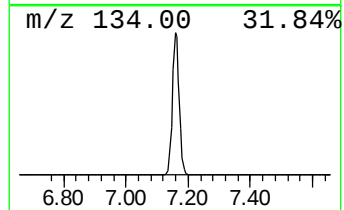
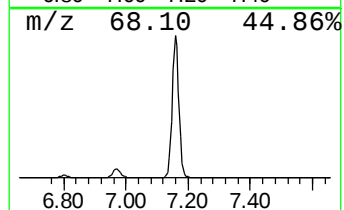
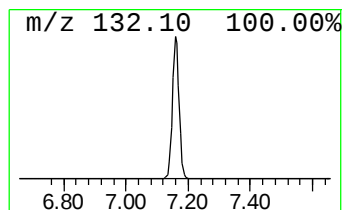
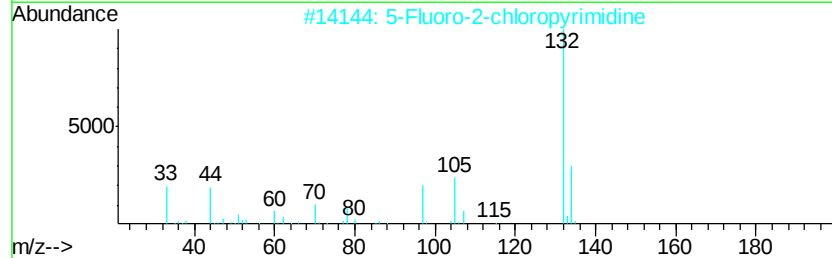
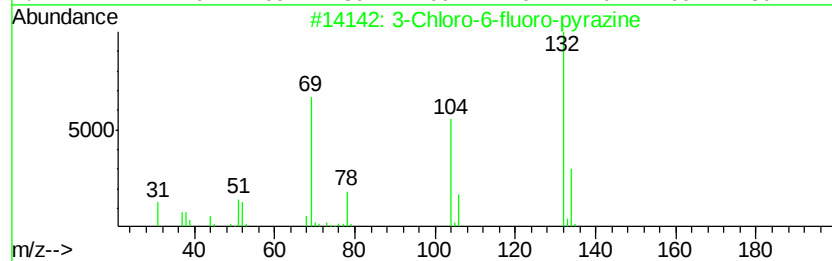
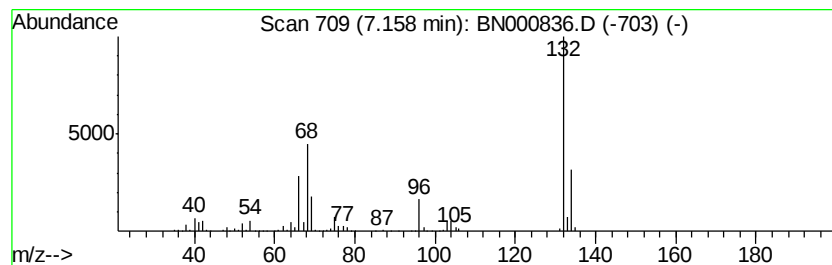
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	22.24 ng/ul	1003230	1,4-Dichlorobenzene-d4	7.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Xenon	132	Xe	007440-63-3	9



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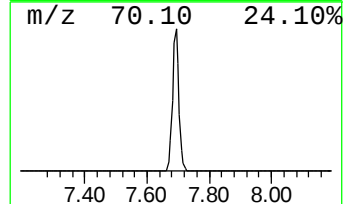
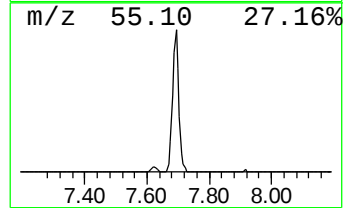
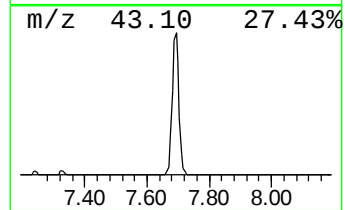
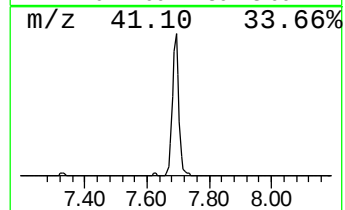
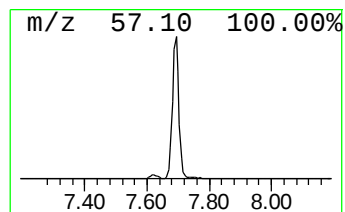
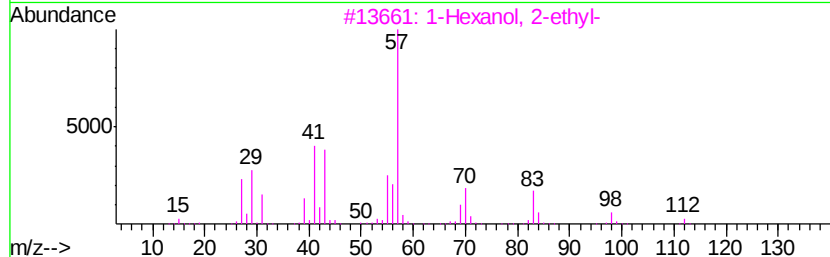
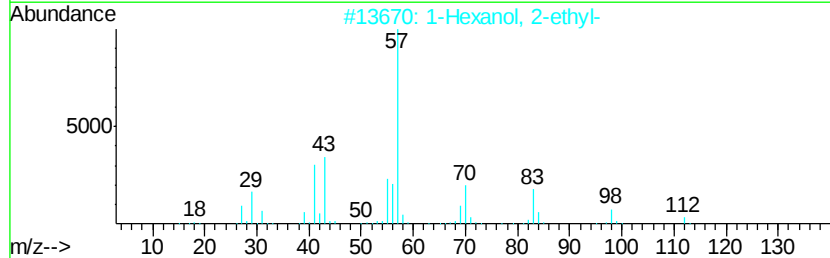
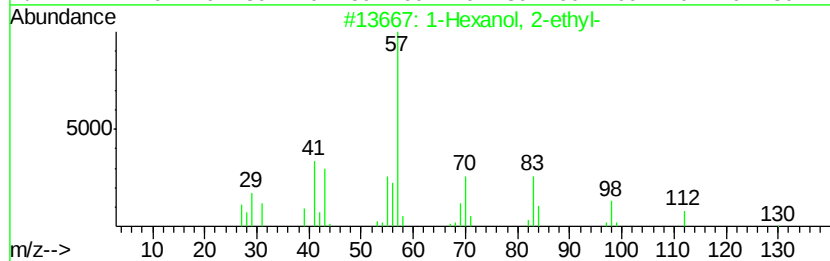
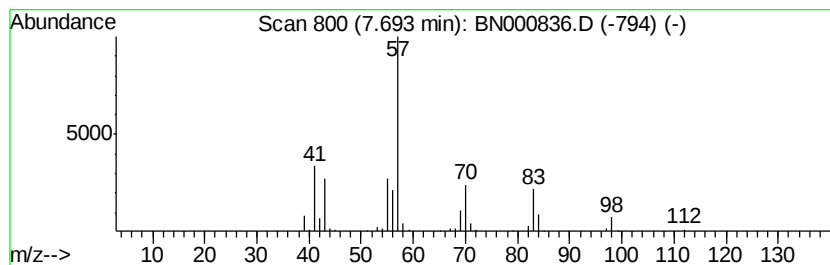
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	6.38 ng/ul	287849	1,4-Dichlorobenzene-d4	7.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



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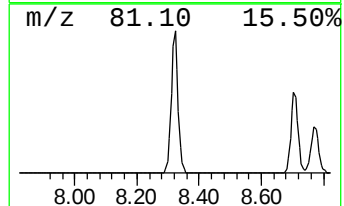
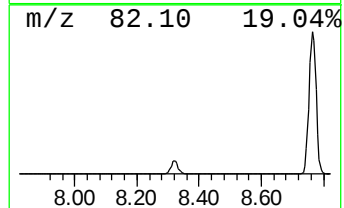
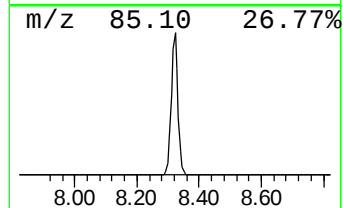
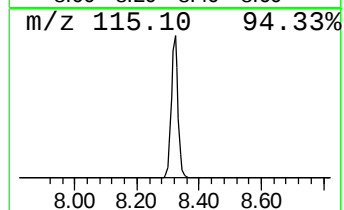
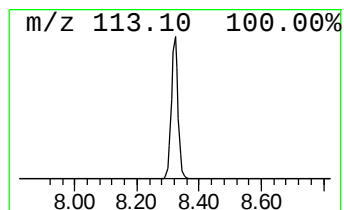
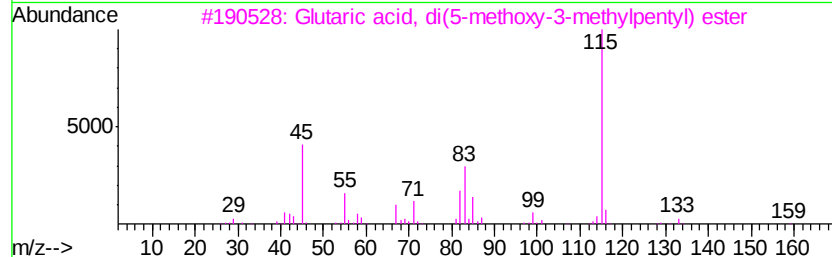
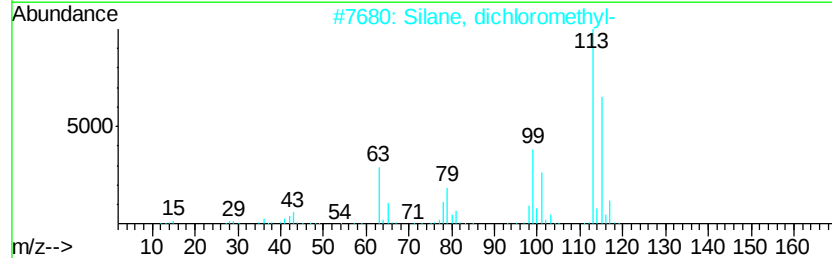
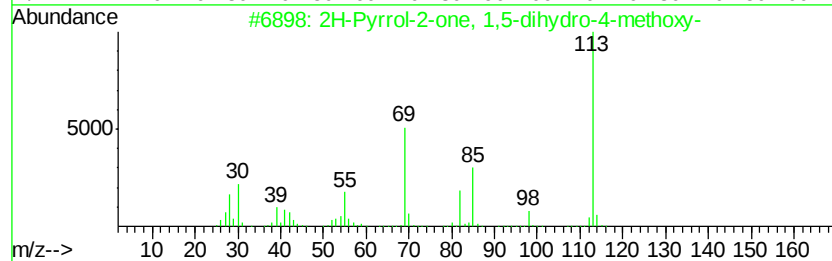
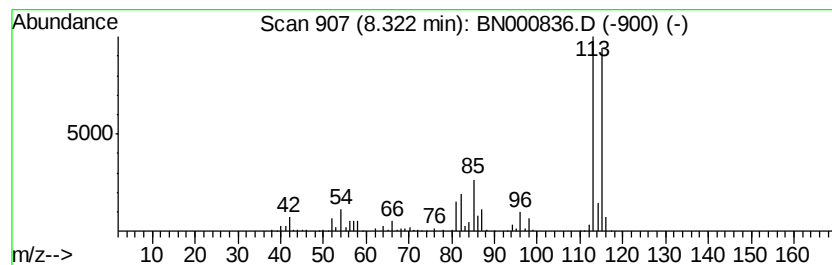
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	18.95 ng/ul	854632	1,4-Dichlorobenzene-d4	7.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	37
2		Silane, dichloromethyl-	114	CH4Cl2Si	000075-54-7	36
3		Glutaric acid, di(5-methoxy-3-me...	360	C19H36O6	1000360-08-3	23
4		Piperidine-2,5-dione	113	C5H7NO2	052065-78-8	17
5		Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	16



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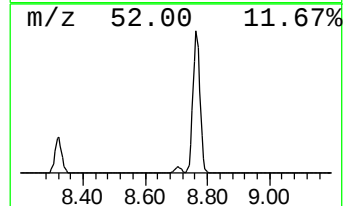
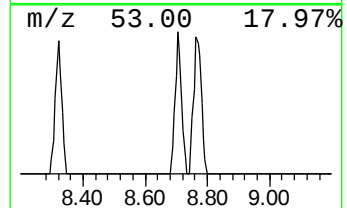
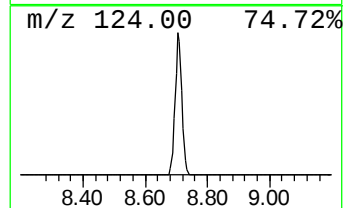
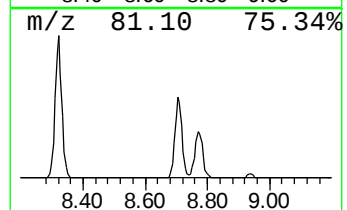
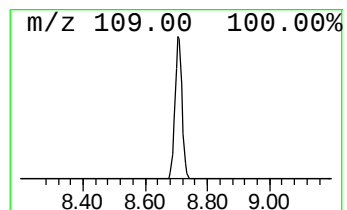
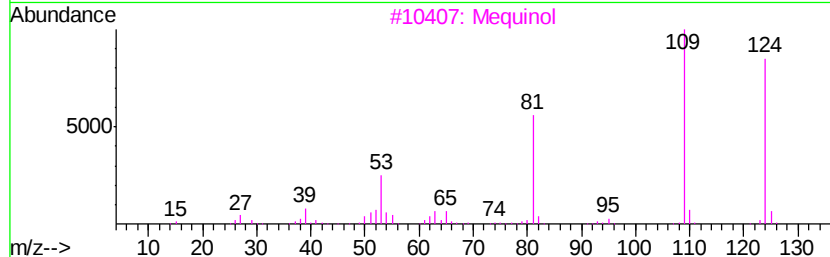
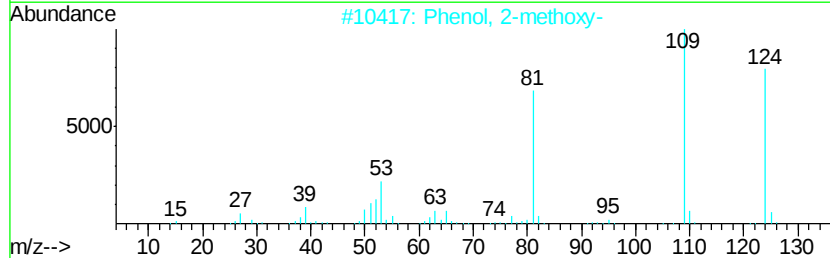
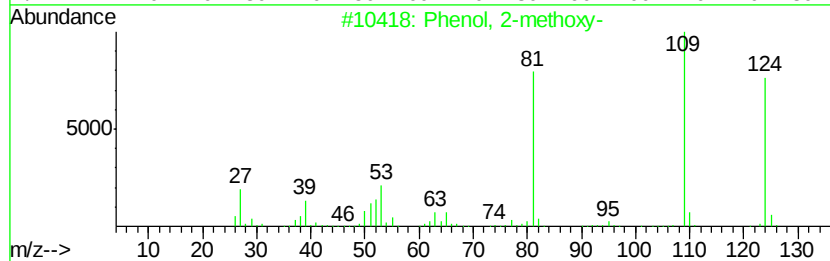
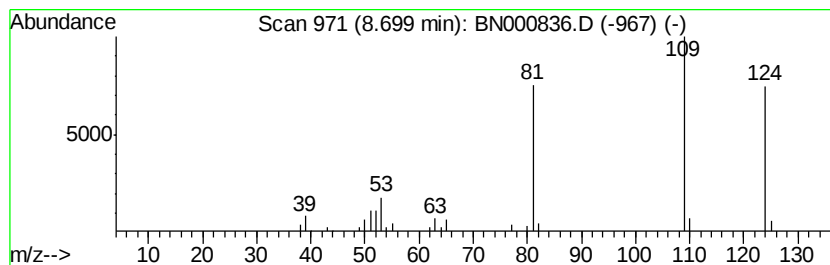
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Phenol, 2-methoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	2.06 ng/ul	92886	1,4-Dichlorobenzene-d4	7.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-			124	C7H8O2	000090-05-1	97
2	Phenol, 2-methoxy-			124	C7H8O2	000090-05-1	97
3	Mequinol			124	C7H8O2	000150-76-5	91
4	Phenol, 2-methoxy-			124	C7H8O2	000090-05-1	90
5	Mequinol			124	C7H8O2	000150-76-5	87



Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000836.D
Acq On : 23 Apr 2018 20:26
Operator : JU/SJ
Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

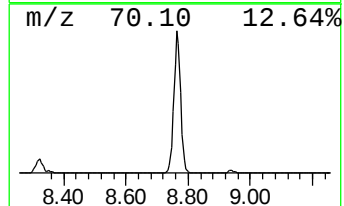
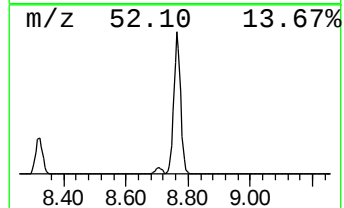
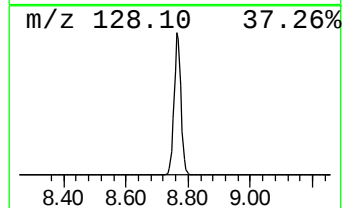
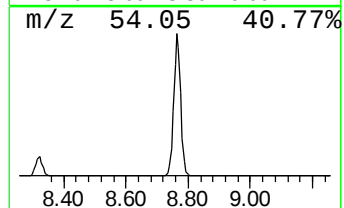
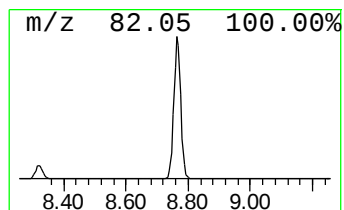
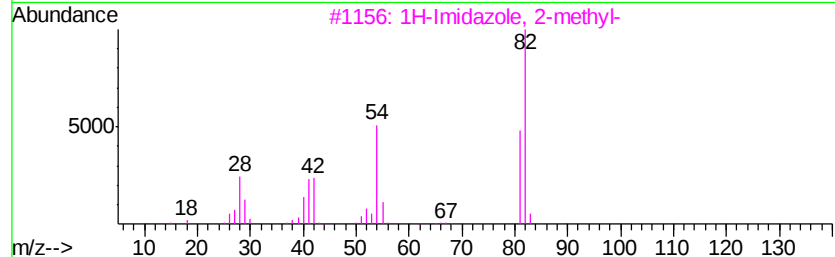
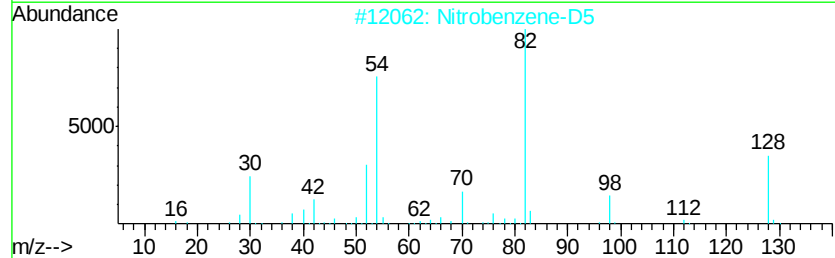
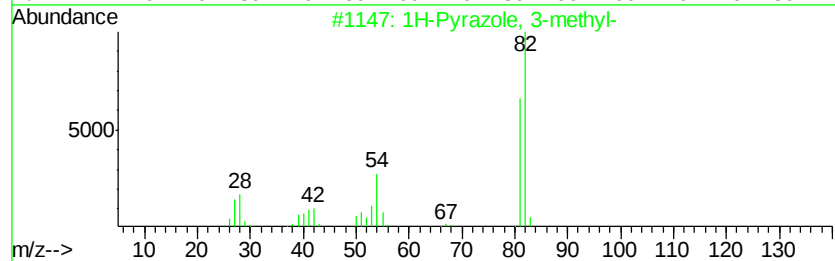
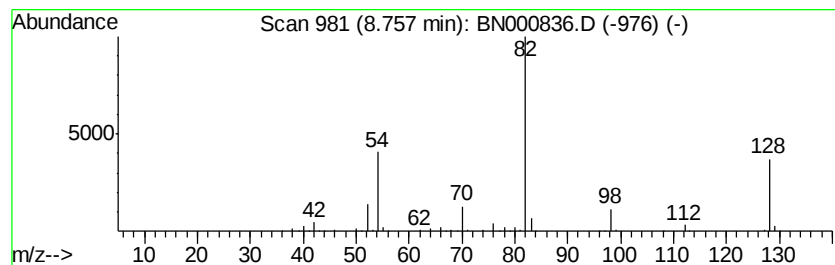
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 1H-Pyrazole, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.76	25.26 ng/ul	1139540	1,4-Dichlorobenzene-d4	7.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
2		Nitrobenzene-D5	128	C6D5NO2	004165-60-0	38
3		1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	33
4		2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	28
5		1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	28



Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000836.D
Acq On : 23 Apr 2018 20:26
Operator : JU/SJ
Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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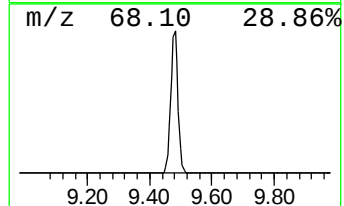
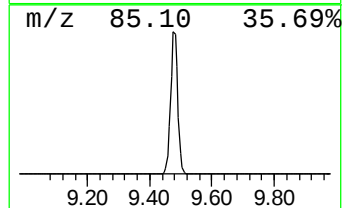
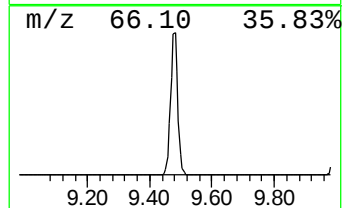
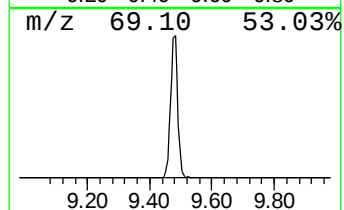
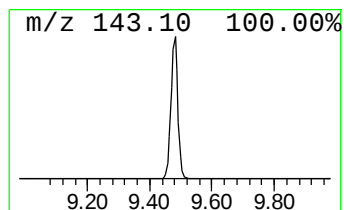
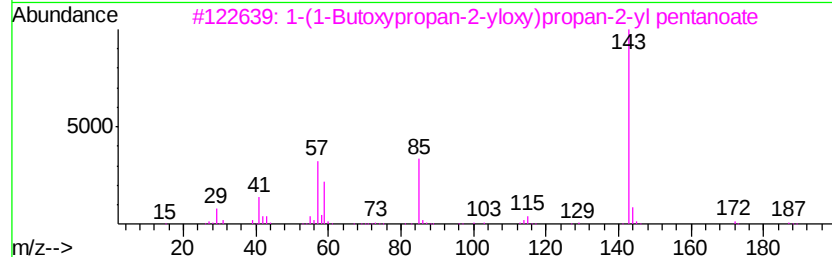
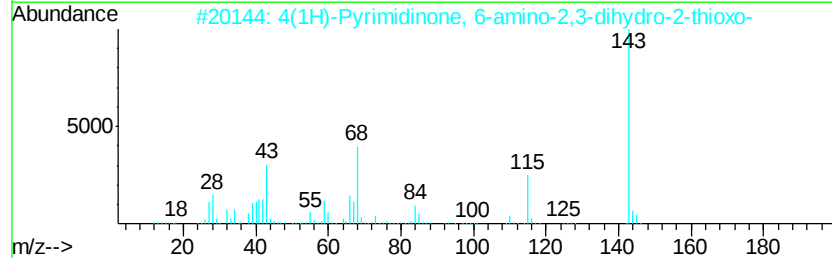
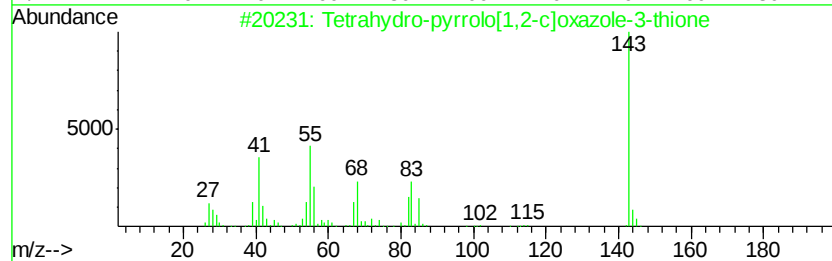
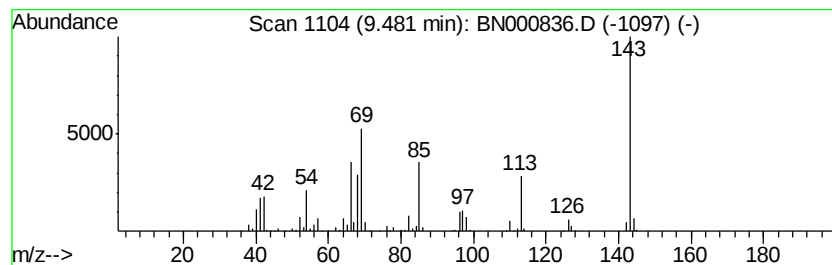
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	13.86 ng/ul	941421	Naphthalene-d8	10.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrahydro-pyrrolo[1,2-c]oxazole...	143	C6H9NOS	1000190-53-6	25
2		4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	17
3		1-(1-Butoxypropan-2-yloxy)propan...	274	C15H30O4	1000367-13-0	12
4		6-Chloro-N-methyl-3-pyridazinamine	143	C5H6ClN3	014959-32-1	12
5		4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	10



Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000836.D
Acq On : 23 Apr 2018 20:26
Operator : JU/SJ
Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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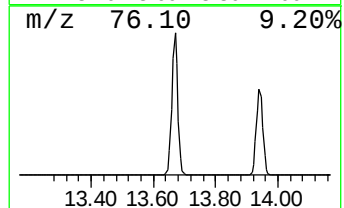
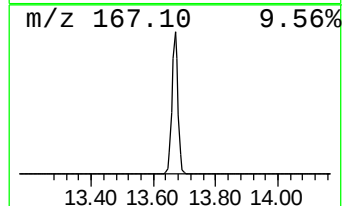
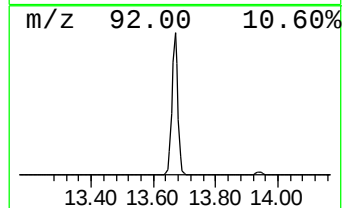
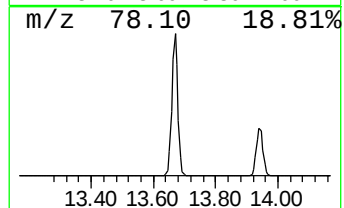
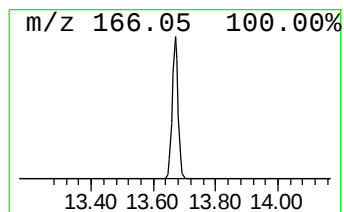
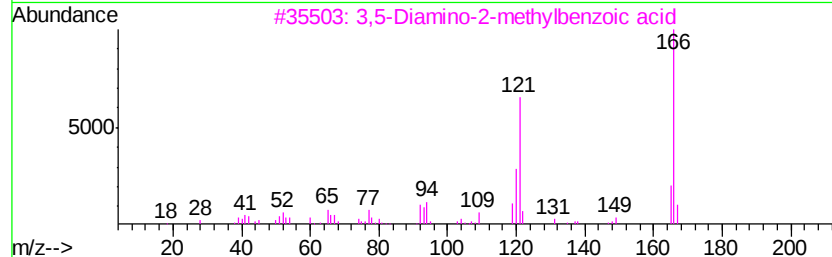
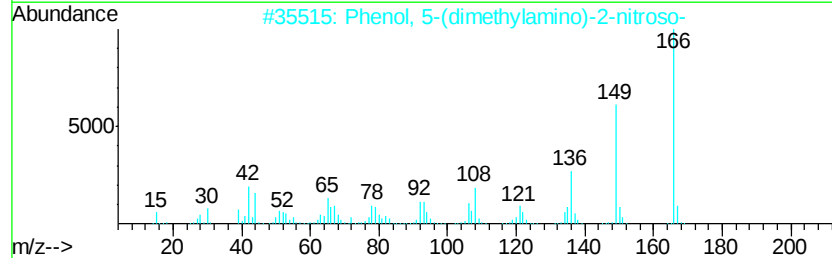
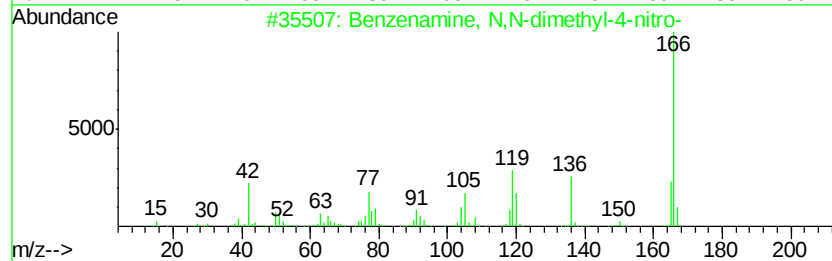
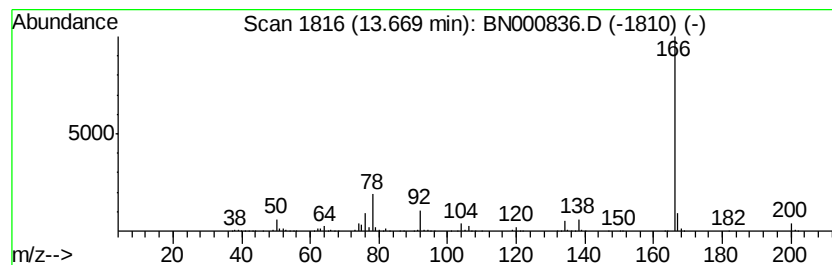
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	24.56 ng/ul	2075540	Acenaphthene-d10	14.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenamine, N,N-dimethyl-4-nitro-	166	C8H10N2O2	000100-23-2	38
2		Phenol, 5-(dimethylamino)-2-nitr...	166	C8H10N2O2	016761-04-9	36
3		3,5-Diamino-2-methylbenzoic acid	166	C8H10N2O2	090007-30-0	36
4		6H-Purine-6-thione, 1,7-dihydro-...	166	C6H6N4S	001126-23-4	9
5		1,3-Benzodioxole-5-carboxylic acid	166	C8H6O4	000094-53-1	9



Data Path : Z:\HPCHEM1\BNA_N\DATA\BN042318\
Data File : BN000836.D
Acq On : 23 Apr 2018 20:26
Operator : JU/SJ
Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

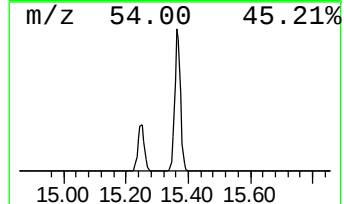
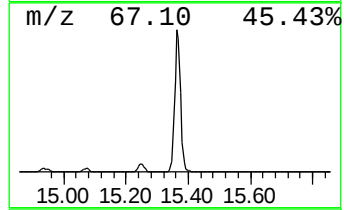
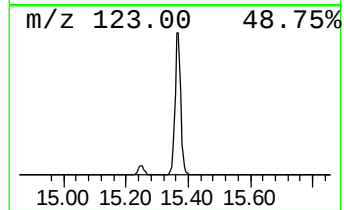
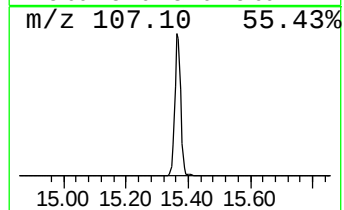
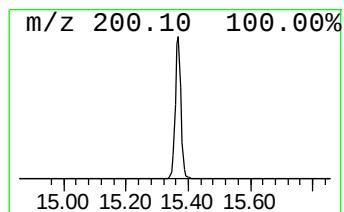
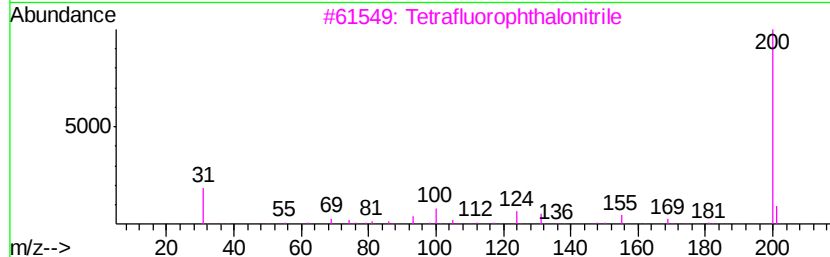
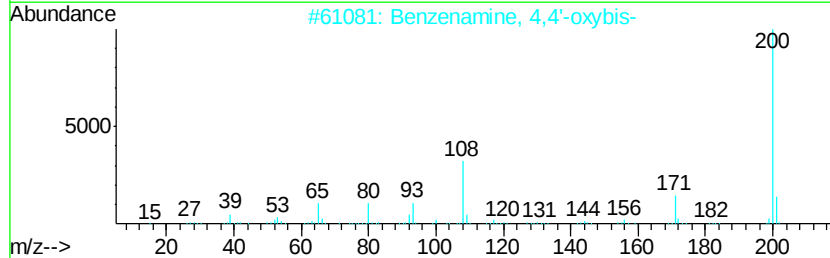
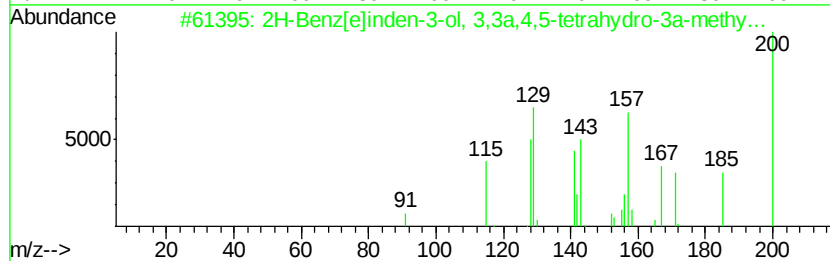
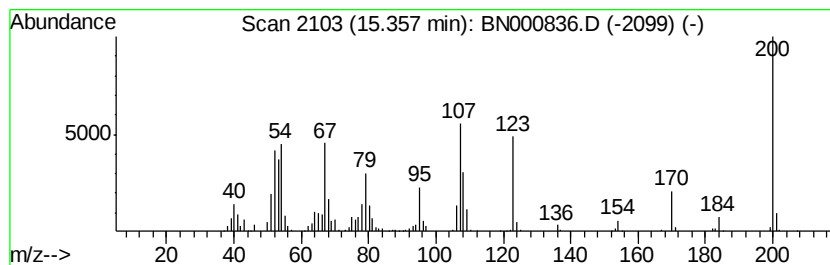
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Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	10.57 ng/ul	893142	Acenaphthene-d10	14.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2H-Benz[e]indene-3-ol, 3,3a,4,5-t...	200 C14H16O	071805-91-9	22
2	Benzenamine, 4,4'-oxybis-	200 C12H12N2O	000101-80-4	11
3	Tetrafluorophthalonitrile	200 C8F4N2	001835-65-0	10
4	1,6-Dioxaspiro[4.4]non-3-ene, 2-...	200 C13H12O2	016863-61-9	10
5	l-Isoleucine, N-neopentyloxycarb...	483 C29H57NO4	1000328-13-3	10



Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
Data File : BN000836.D
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Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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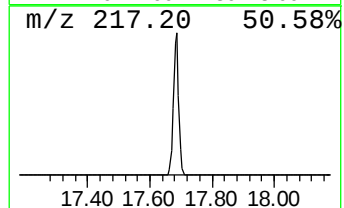
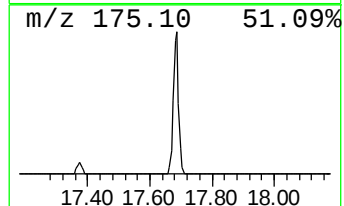
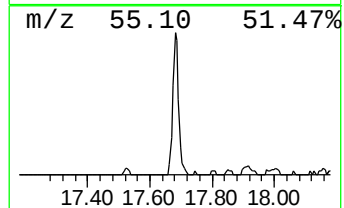
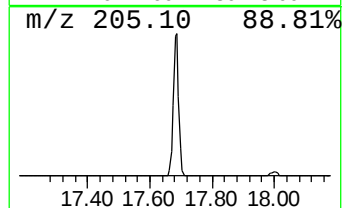
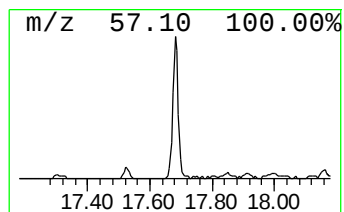
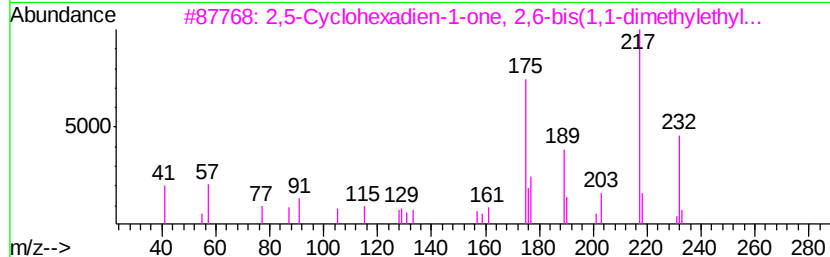
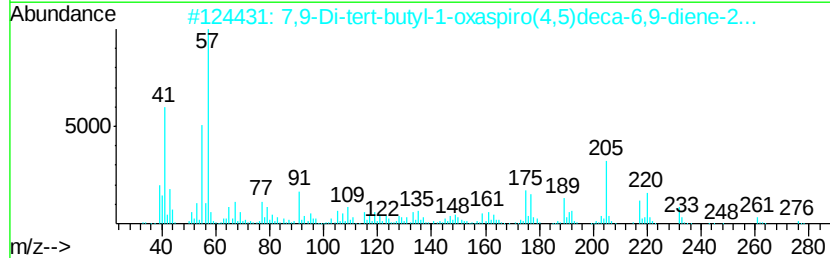
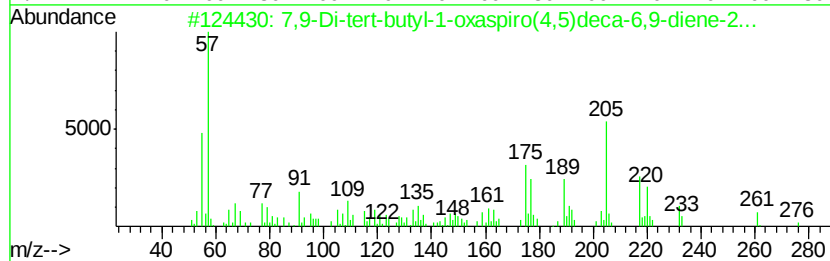
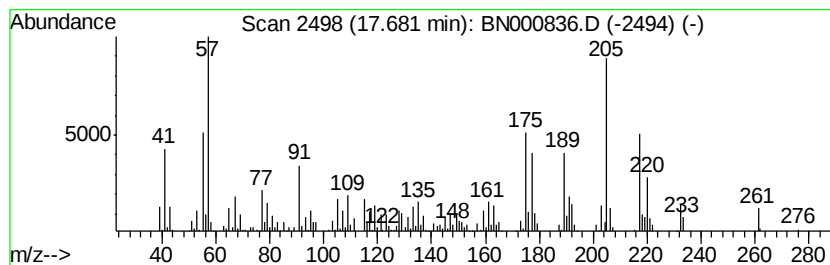
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.68	4.25 ng/ul	391166	Phenanthrene-d10	17.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	99
2			7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2-one	276	C17H24O3	082304-66-3	98
3			2,5-Cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-	232	C16H24O	006738-27-8	83
4			Ethanone, 1-(5,6,7,8-tetrahydro-2H-chromeno[2,1-b]pyridin-2-yl)-	220	C14H20O2	071596-88-8	50
5			2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	42



Data Path : Z:\HPCHEM1\BNA N\DATA\BN042318\
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Acq On : 23 Apr 2018 20:26
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Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

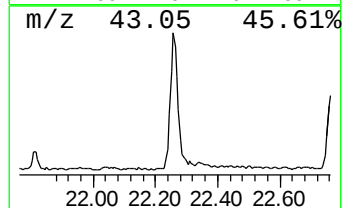
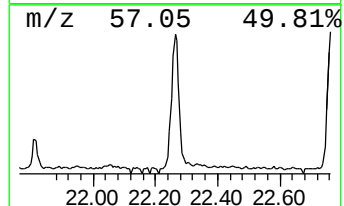
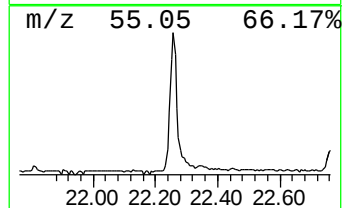
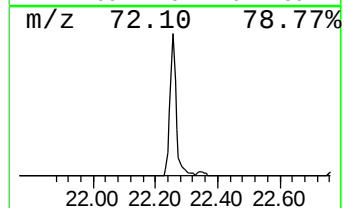
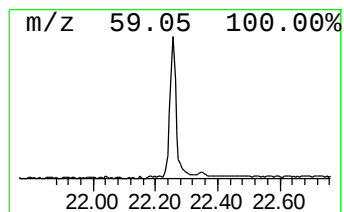
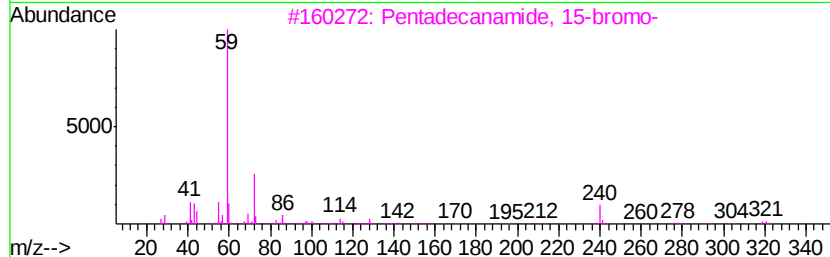
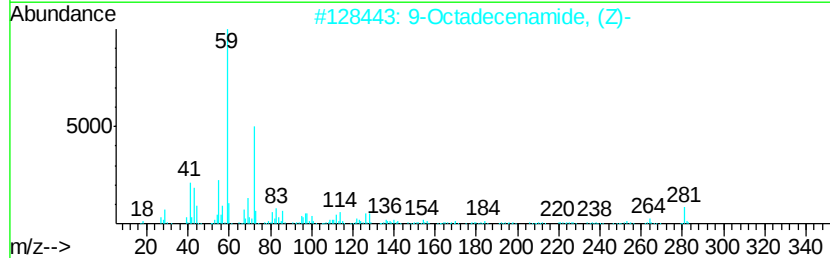
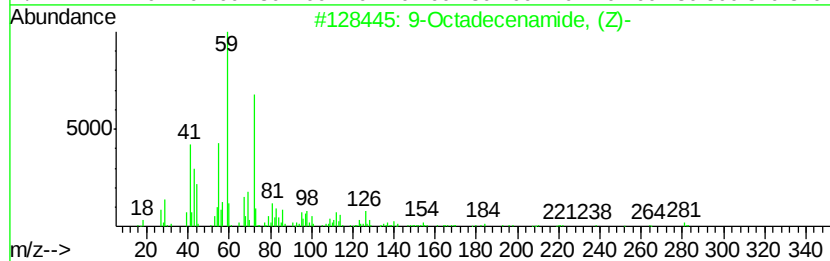
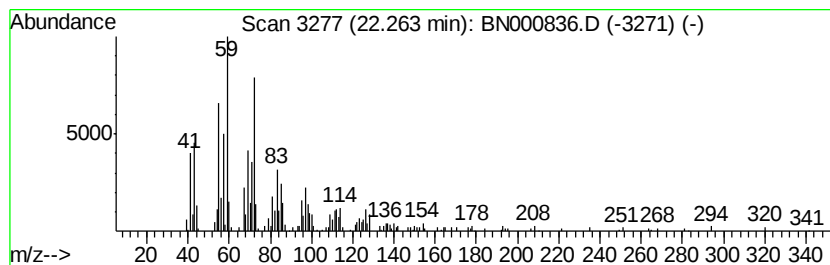
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ClientSampleId :
A3Y06

Quant Method : Z:\HPCHEM1\BNA N\METHODS\SOM-EPA-BN041918-PAH.M
Quant Title : SVOA CALIBRATION

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

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.26	4.48 ng/ul	367822	Chrysene-d12	21.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	90
2	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	64
3	Pentadecanamide, 15-bromo-	319 C15H30BrNO	1000163-86-1	53
4	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	47
5	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	47



Data Path : Z:\HPCHEM1\BNA_N\DATA\BN042318\
Data File : BN000836.D
Acq On : 23 Apr 2018 20:26
Operator : JU/SJ
Sample : J2467-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
A3Y06

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041918-PAH.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
Cyclohexanone	5.71	2.0	ng/ul	91091	1	7.62	902224	20.0
p-Nitrophenyl hex...	6.80	6.5	ng/ul	295406	1	7.62	902224	20.0
unknown-01	7.16	22.2	ng/ul	1003230	1	7.62	902224	20.0
1-Hexanol, 2-ethyl-	7.69	6.4	ng/ul	287849	1	7.62	902224	20.0
unknown-02	8.32	18.9	ng/ul	854632	1	7.62	902224	20.0
Phenol, 2-methoxy-	8.70	2.1	ng/ul	92886	1	7.62	902224	20.0
1H-Pyrazole, 3-me...	8.76	25.3	ng/ul	1139540	1	7.62	902224	20.0
unknown-03	9.48	13.9	ng/ul	941421	2	10.39	1358280	20.0
unknown-04	13.67	24.6	ng/ul	2075540	3	14.25	1689970	20.0
unknown-05	15.36	10.6	ng/ul	893142	3	14.25	1689970	20.0
7,9-Di-tert-butyl...	17.68	4.3	ng/ul	391166	4	17.00	1840680	20.0
9-Octadecenamide, ...	22.26	4.5	ng/ul	367822	5	21.20	1641690	20.0