

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
 Data File : BG036798.D
 Acq On : 18 Sep 2018 23:03
 Operator : JU/SJ
 Sample : J4922-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PZ-6

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % 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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.620	389	397	409	rVB	395933	641182	15.93%	3.308%
2	7.200	658	666	681	rBV	261187	463718	11.52%	2.393%
3	7.576	719	730	738	rBV	719131	1236914	30.73%	6.382%
4	8.046	804	810	817	rBV	177974	293636	7.30%	1.515%
5	8.369	858	865	878	rVB	602256	1040013	25.84%	5.366%
6	9.210	1000	1008	1016	rBV	580949	1023013	25.42%	5.278%
7	10.561	1230	1238	1245	rBV5	17521	44031	1.09%	0.227%
8	10.855	1279	1288	1298	rVB	253601	468703	11.64%	2.418%
9	11.701	1417	1432	1437	rBV7	31804	86813	2.16%	0.448%
10	12.588	1575	1583	1586	rBV6	22345	53242	1.32%	0.275%
11	12.788	1609	1617	1627	rVB10	38837	124631	3.10%	0.643%
12	13.076	1661	1666	1672	rVB6	29038	54377	1.35%	0.281%
13	13.193	1679	1686	1695	rVB9	28223	81036	2.01%	0.418%
14	13.299	1695	1704	1710	rBV	1450002	2350475	58.40%	12.128%
15	13.622	1755	1759	1762	rBV5	25046	46031	1.14%	0.238%
16	13.693	1767	1771	1774	rBV5	29941	45842	1.14%	0.237%
17	13.787	1783	1787	1792	rBV4	34635	51084	1.27%	0.264%
18	13.910	1804	1808	1814	rVB7	35952	61337	1.52%	0.316%
19	14.004	1820	1824	1827	rBV4	37036	54966	1.37%	0.284%
20	14.310	1873	1876	1884	rVB5	51109	81963	2.04%	0.423%
21	14.492	1900	1907	1920	rBV5	32972	131073	3.26%	0.676%
22	14.603	1921	1926	1932	rBV10	27178	59812	1.49%	0.309%
23	14.674	1932	1938	1945	rBV2	440928	724677	18.00%	3.739%
24	14.733	1945	1948	1951	rBV3	44311	64668	1.61%	0.334%
25	15.156	2016	2020	2023	rBV5	55429	82454	2.05%	0.425%
26	15.320	2042	2048	2054	rVB7	80618	180491	4.48%	0.931%
27	15.714	2111	2115	2121	rBV3	61461	108887	2.71%	0.562%
28	15.778	2122	2126	2130	rVV5	30113	49559	1.23%	0.256%
29	16.160	2185	2191	2202	rBV	1374166	2160882	53.68%	11.150%
30	17.418	2399	2405	2413	rVB	596622	920230	22.86%	4.748%
31	18.305	2552	2556	2565	rBV2	84388	141437	3.51%	0.730%
32	19.574	2768	2772	2777	rBV3	52290	75247	1.87%	0.388%
33	20.026	2843	2849	2855	rBV	3122902	4025122	100.00%	20.769%
34	20.902	2994	2998	3003	rVB	141461	177736	4.42%	0.917%

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Stop Thrs : 0 Peak Location: TOP

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35	21.683	3125	3131	3139	rVB2	667164	1065759	26.48%	5.499%
36	24.891	3668	3677	3689	rVB2	386562	1109771	27.57%	5.726%

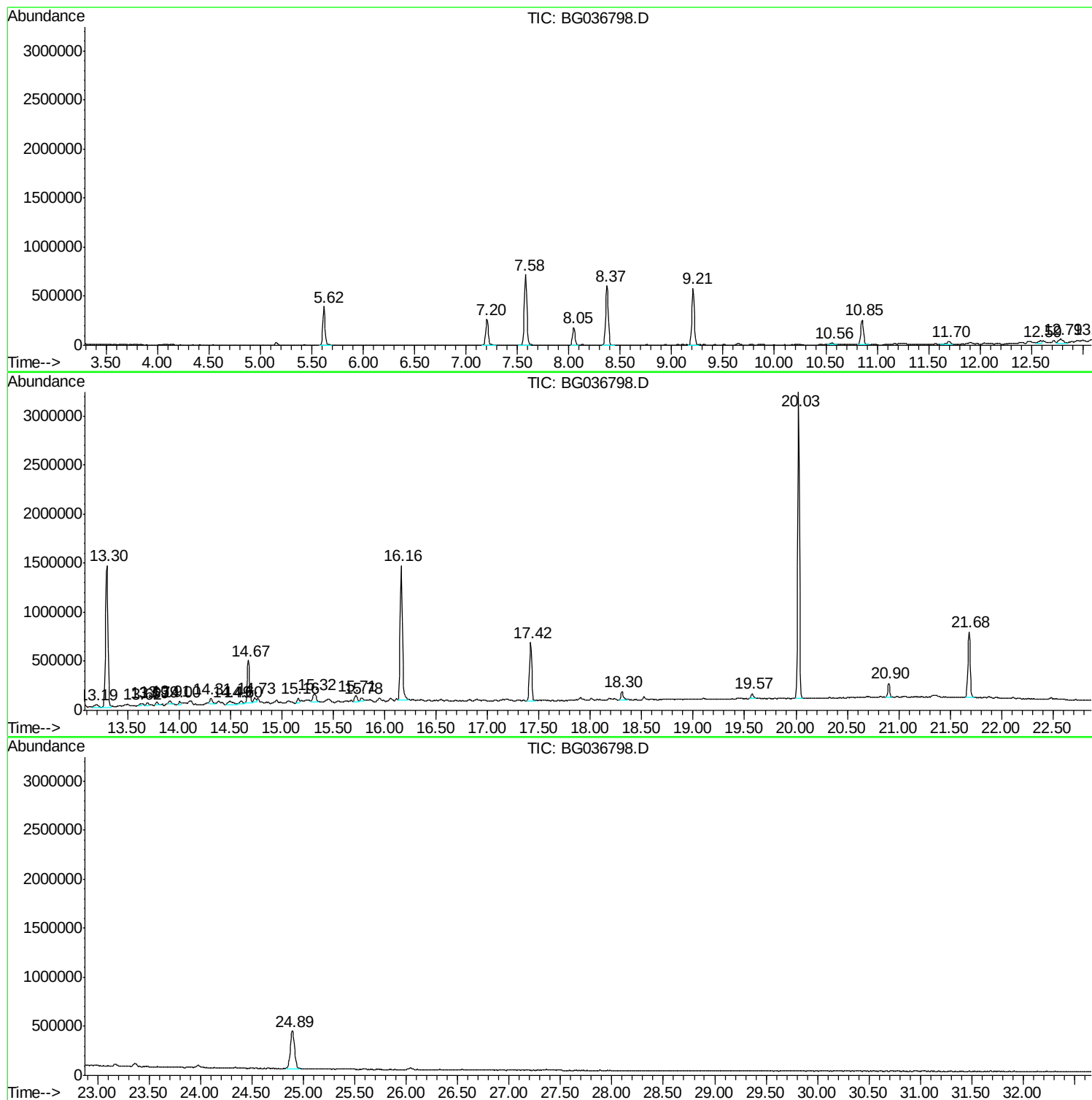
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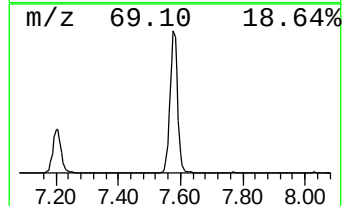
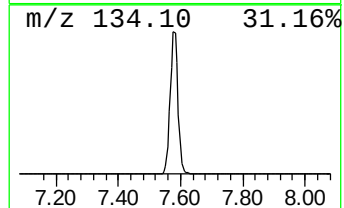
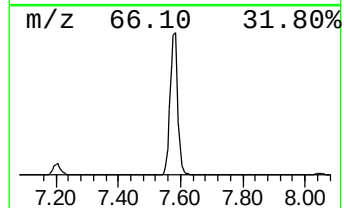
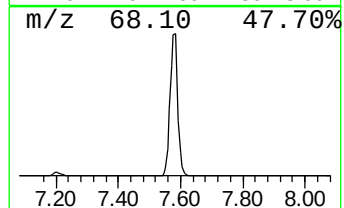
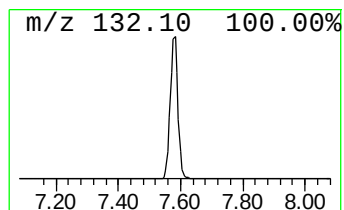
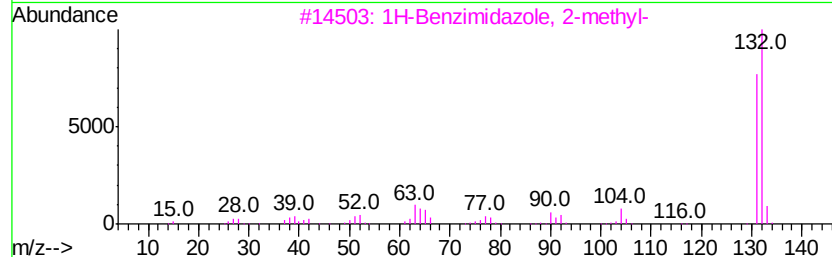
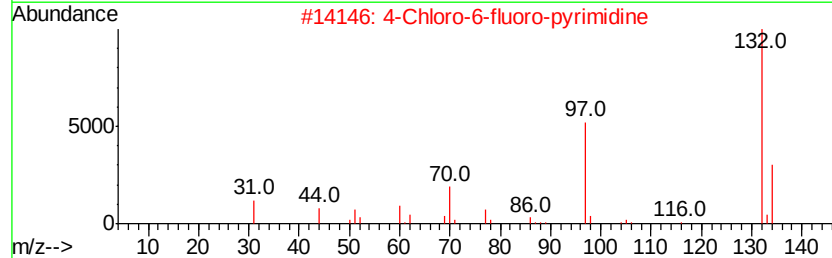
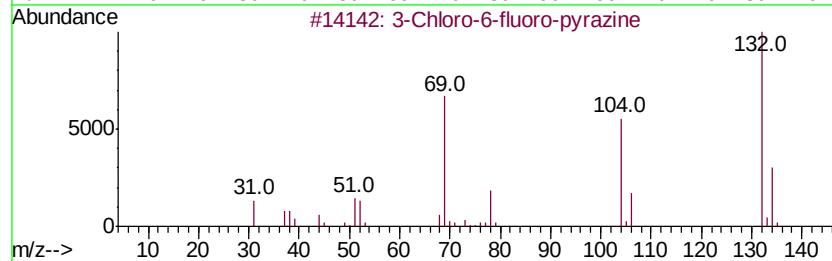
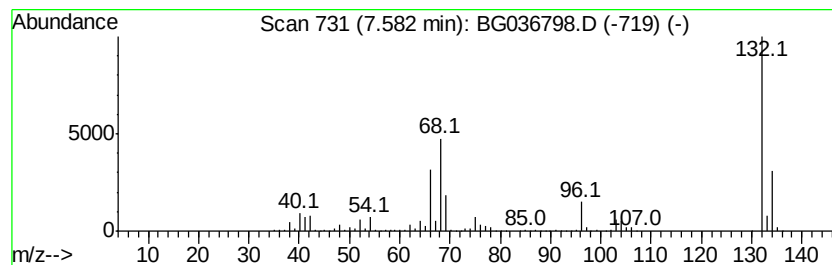
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TIC Library : C:\Database\NIST11.L
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Peak Number 1 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	84.25 ng	1236910	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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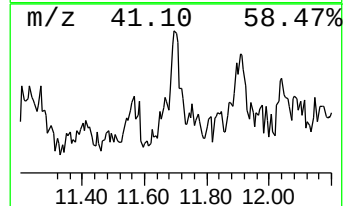
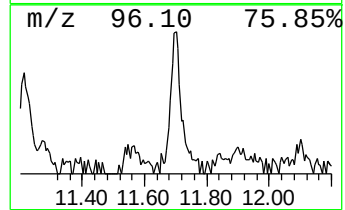
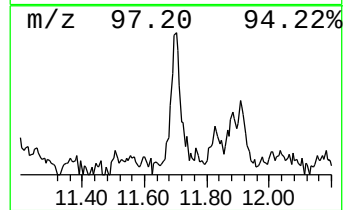
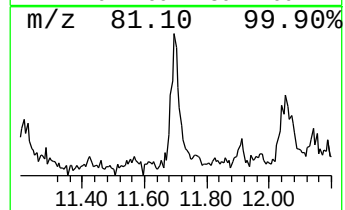
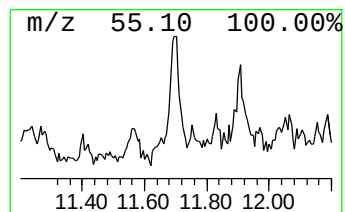
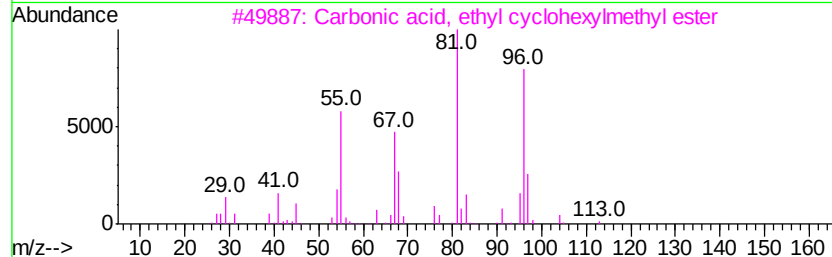
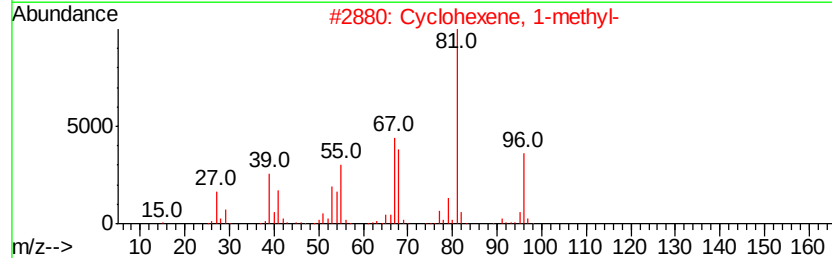
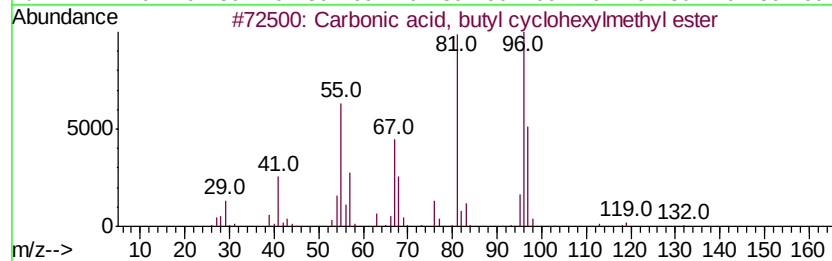
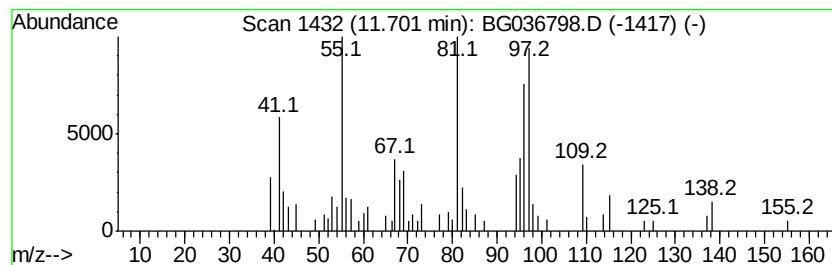
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Peak Number 3 unknown11.70 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.70	3.70 ng	86813	Napthalene-d8	10.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, butyl cyclohexylm...	214	C12H22O3	1000357-84-5	47
2	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	43
3	Carbonic acid, ethyl cyclohexylm...	186	C10H18O3	1000357-91-5	43
4	1H-Imidazol, 1-methyl-2-amino-	97	C4H7N3	006646-51-1	43
5	trans-2-Methylcyclohexanol, pent...	260	C10H13F5O2	1000364-13-4	43



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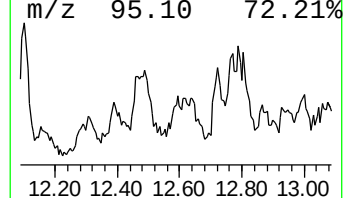
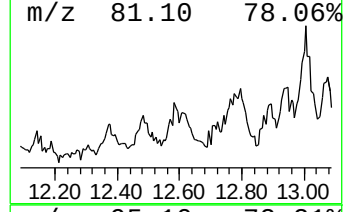
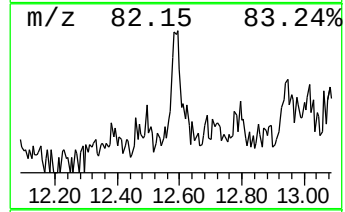
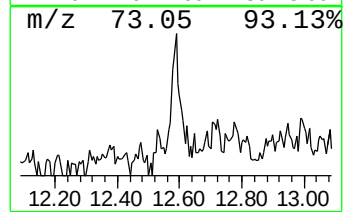
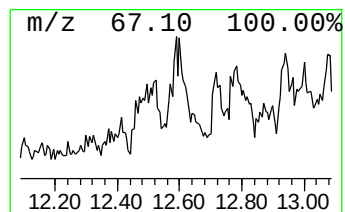
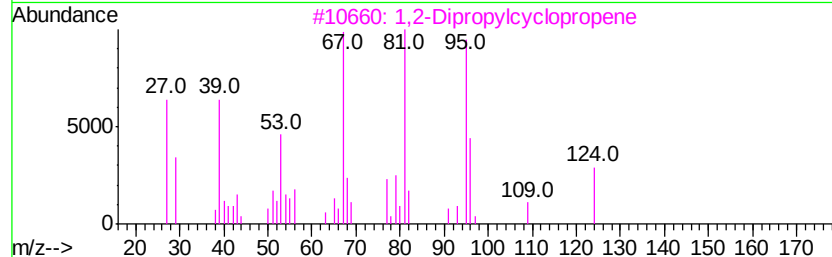
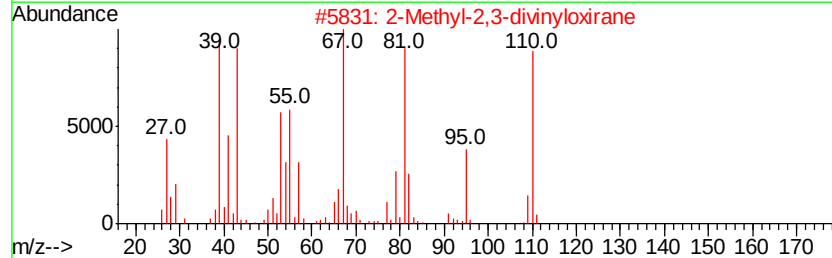
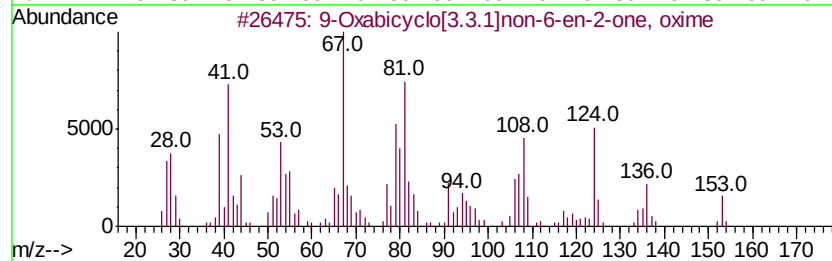
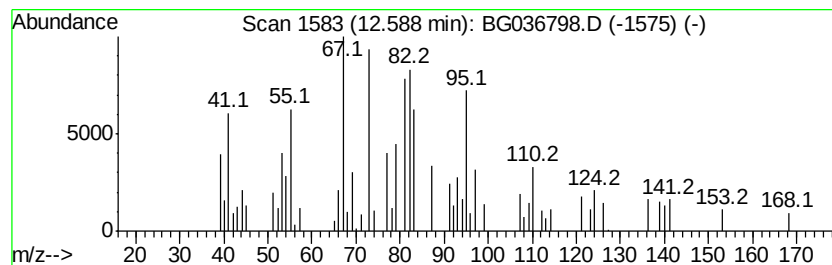
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Peak Number 4 9-Oxabicyclo[3.3.1]non-6-en... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.27 ng	53242	Naphthalene-d8	10.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		9-Oxabicyclo[3.3.1]non-6-en-2-on...	153 C8H11NO2	063827-16-7 70
2		2-Methyl-2,3-divinyloxirane	110 C7H10O	070597-50-1 64
3		1,2-Dipropylcyclopropene	124 C9H16	010306-92-0 49
4		2-Hexyne	82 C6H10	000764-35-2 43
5		4-Nonyne	124 C9H16	020184-91-2 43



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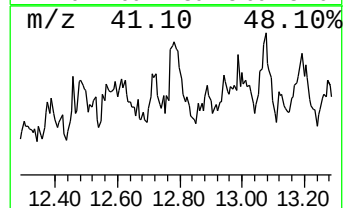
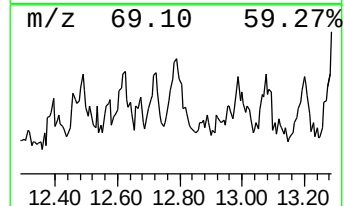
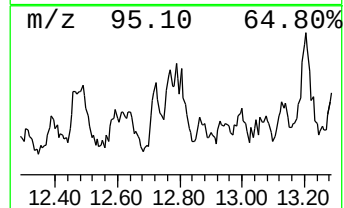
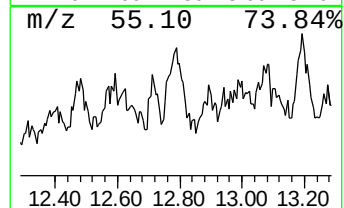
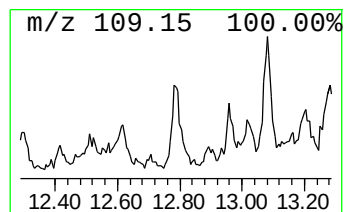
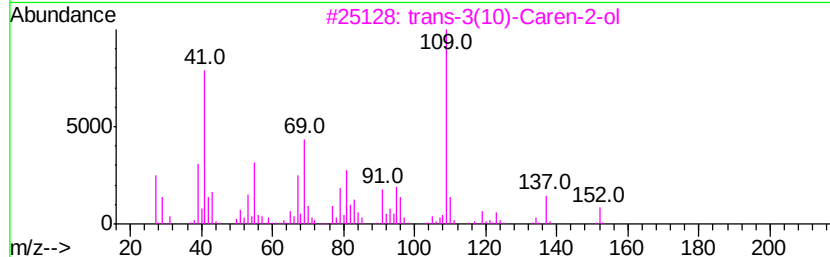
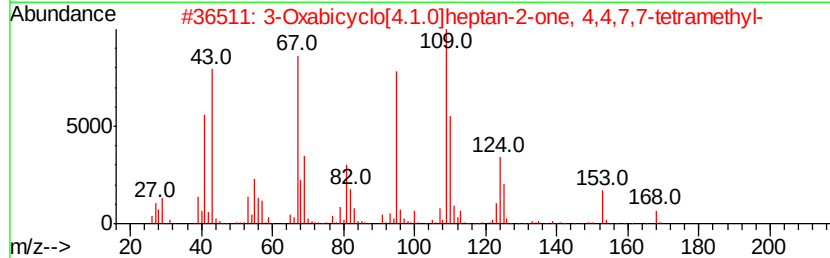
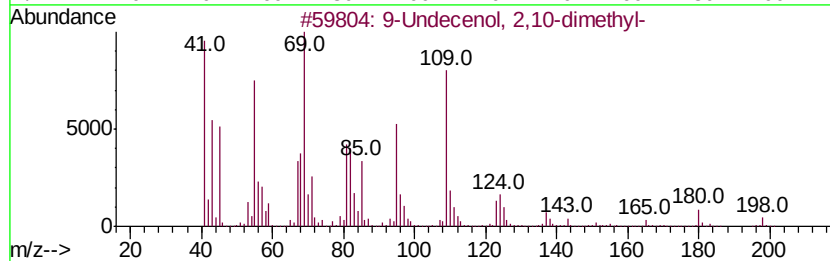
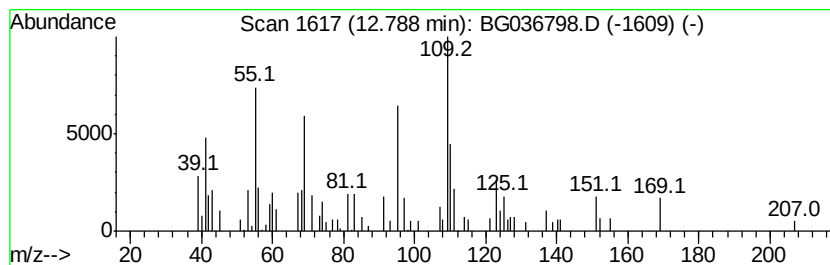
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Peak Number 5 9-Undecenol, 2,10-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	3.44 ng	124631	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	50
2		3-Oxabicyclo[4.1.0]heptan-2-one,...	168	C10H16O2	022841-82-3	42
3		trans-3(10)-Caren-2-ol	152	C10H16O	1000151-66-5	38
4		Benzene, 1-fluoro-2-methyl-	110	C7H7F	000095-52-3	25
5		trans-2-Caren-4-ol	152	C10H16O	004017-82-7	25



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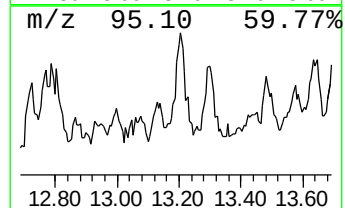
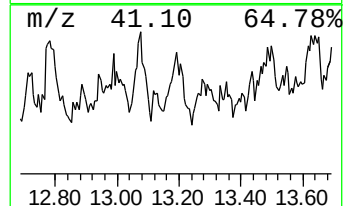
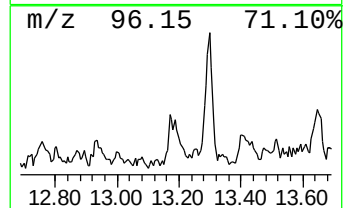
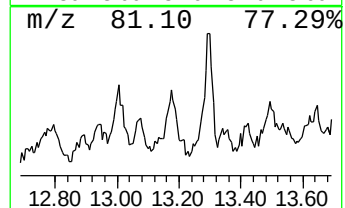
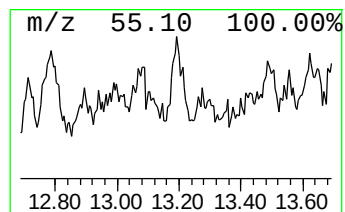
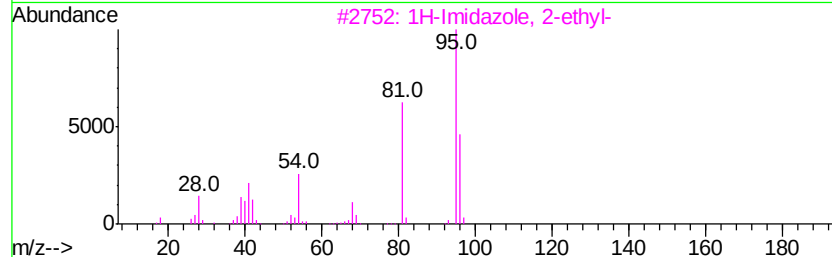
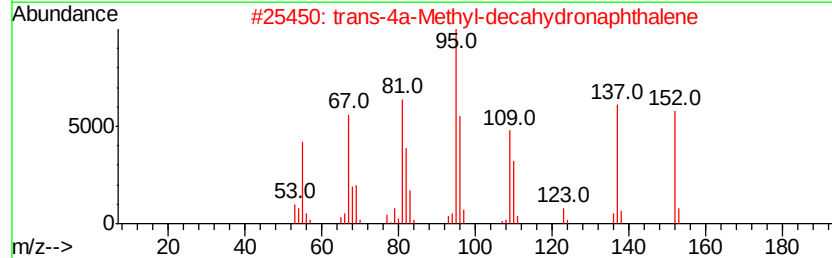
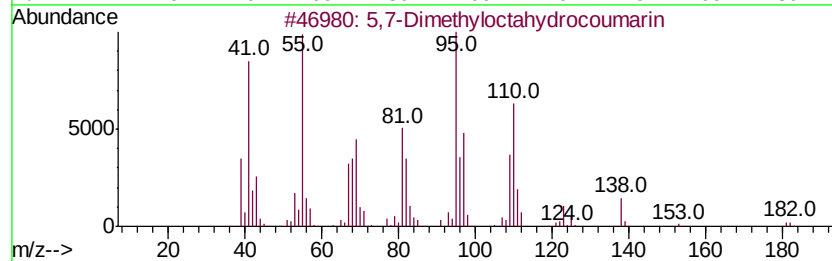
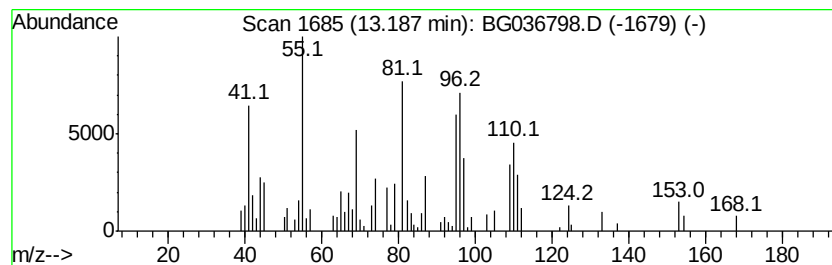
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Peak Number 6 unknown13.19 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.24 ng	81036	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5,7-Dimethyloctahydrocoumarin	182	C11H18O2	1000109-81-5	42
2		trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	40
3		1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	38
4		5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	35
5		1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	35



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Operator : JU/SJ
Sample : J4922-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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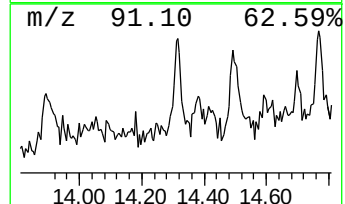
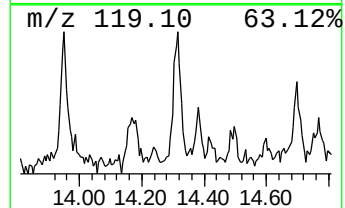
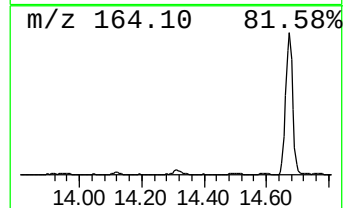
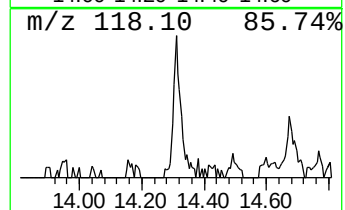
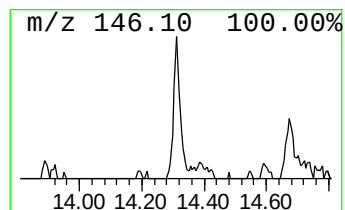
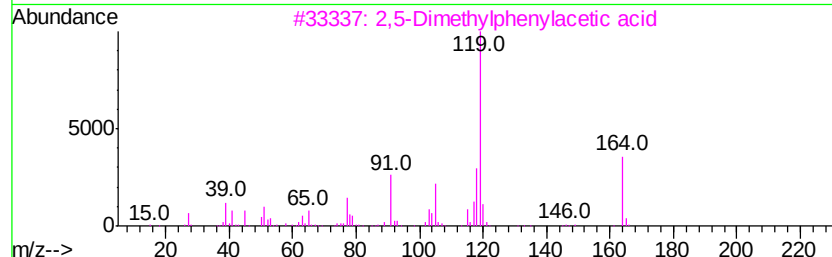
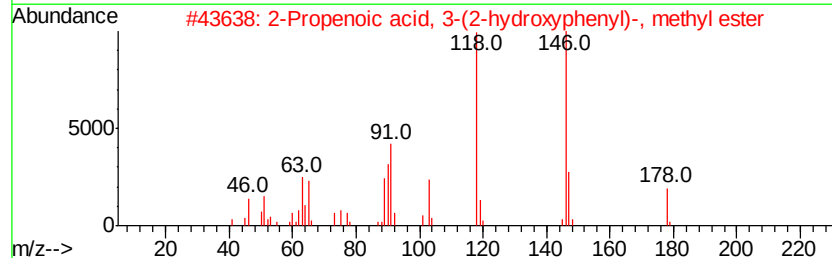
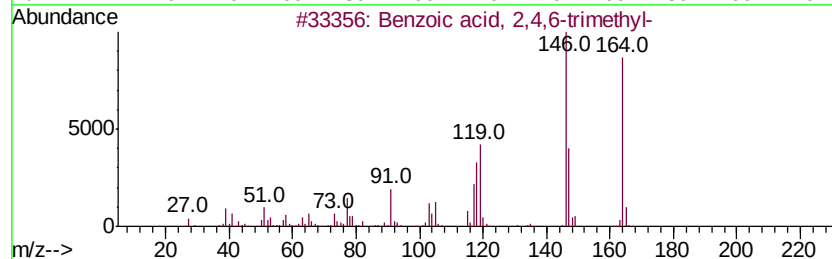
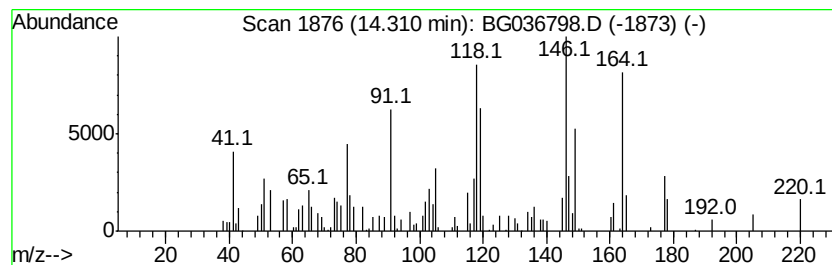
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	2.26 ng	81963	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	60
2		2-Propenoic acid, 3-(2-hydroxyph...	178	C10H10O3	020883-98-1	46
3		2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	38
4		2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	30
5		Benzoimidazole-1-carbaldehyde	146	C8H6N2O	1000294-58-3	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
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ALS Vial : 14 Sample Multiplier: 1

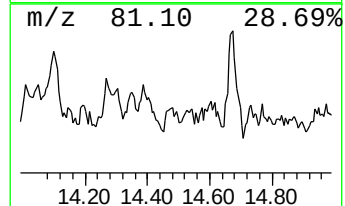
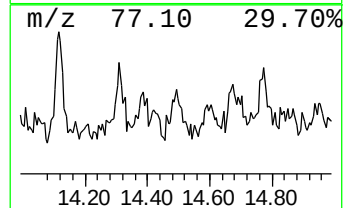
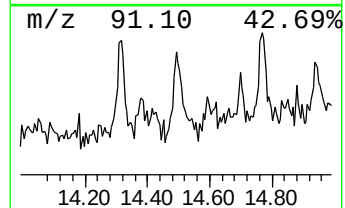
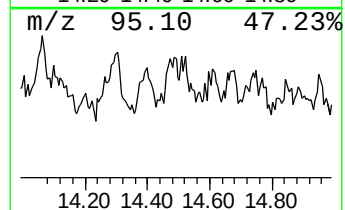
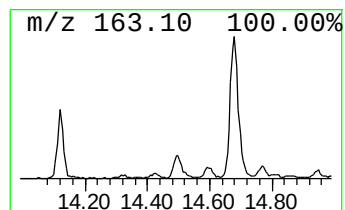
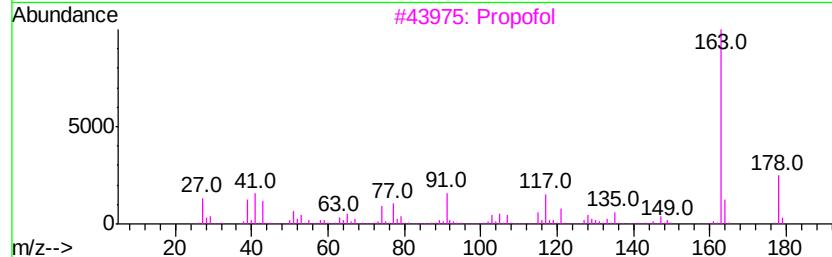
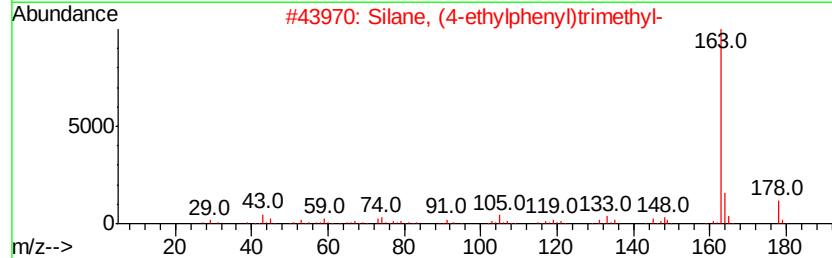
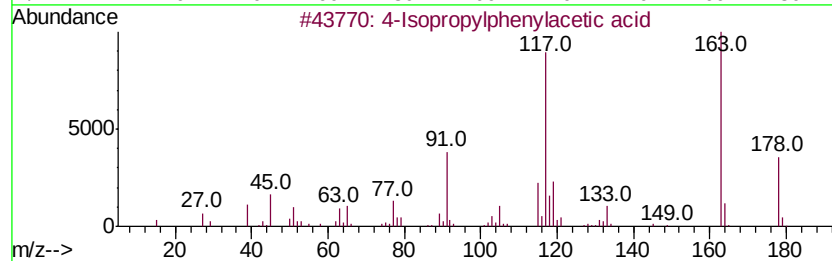
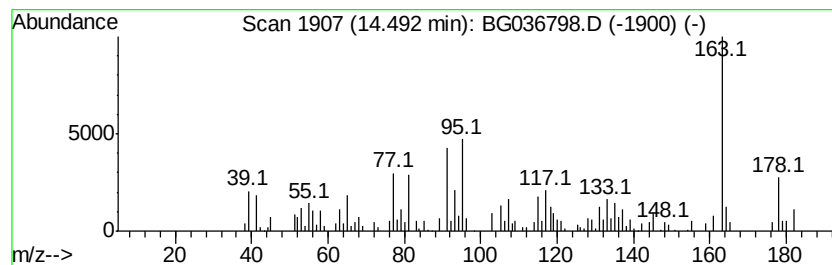
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4-Isopropylphenylacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.49	3.62 ng	131073	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Isopropylphenylacetic acid	178	C11H14O2	004476-28-2	70
2	Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	49
3	Propofol	178	C12H18O	002078-54-8	49
4	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	46
5	1,4-Benzenediamine, N4-,N4-dieth...	178	C11H18N2	000148-71-0	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
Acq On : 18 Sep 2018 23:03
Operator : JU/SJ
Sample : J4922-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

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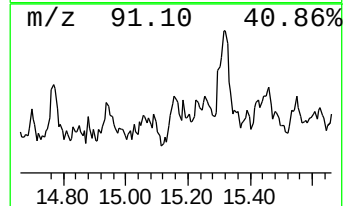
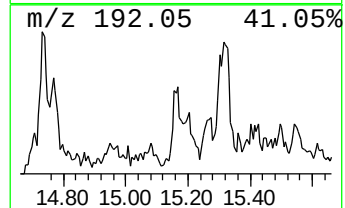
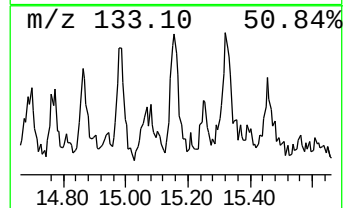
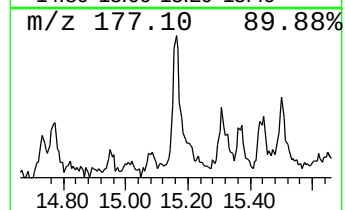
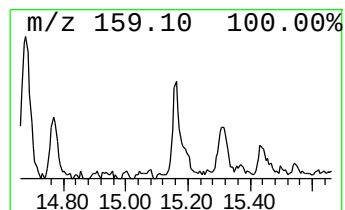
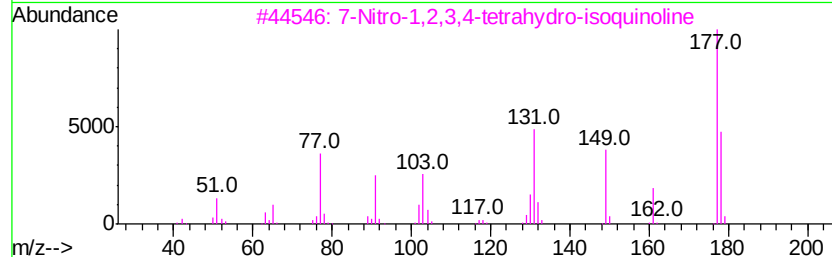
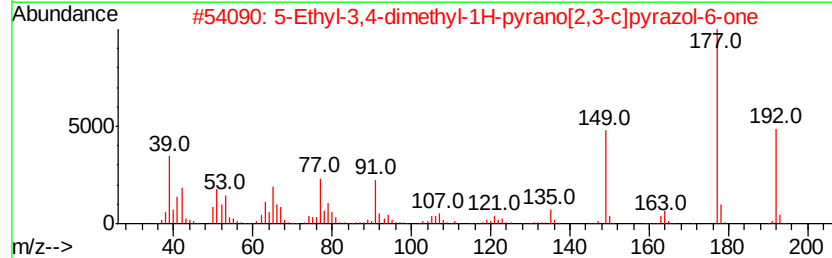
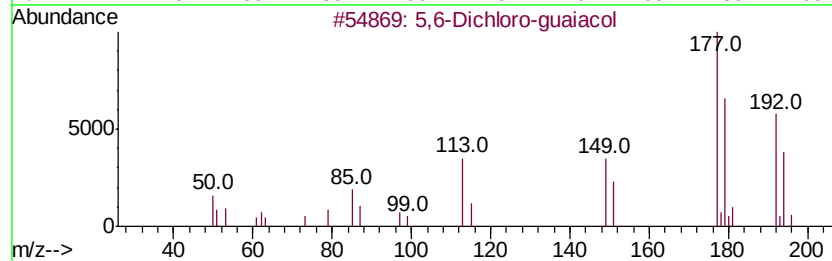
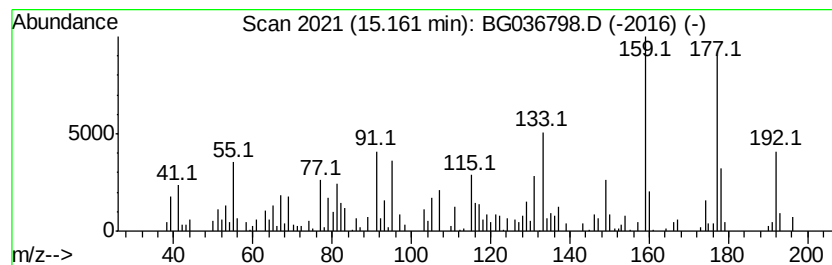
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.16 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.28 ng	82454	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5,6-Dichloro-quaiacol	192	C7H6Cl2O2	077102-95-5	30
2		5-Ethyl-3,4-dimethyl-1H-pyrano[2...	192	C10H12N2O2	1000296-60-7	30
3		7-Nitro-1,2,3,4-tetrahydro-isoqu...	178	C9H10N2O2	1000318-52-7	30
4		Benzoic acid, 2-acetyl-3,6-dimet...	192	C11H12O3	146950-86-9	25
5		2,6-Diisopropylanisole	192	C13H20O	002944-52-7	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
Acq On : 18 Sep 2018 23:03
Operator : JU/SJ
Sample : J4922-05
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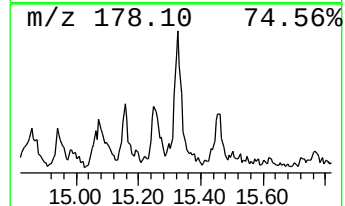
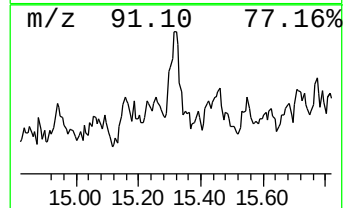
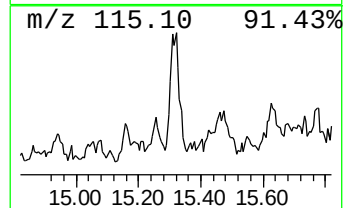
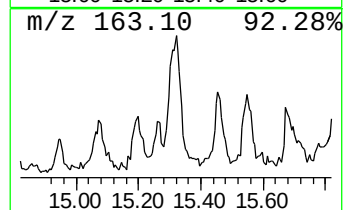
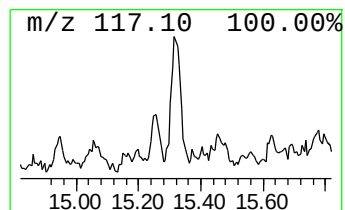
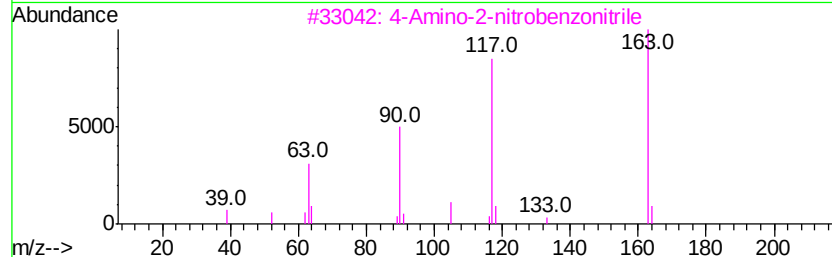
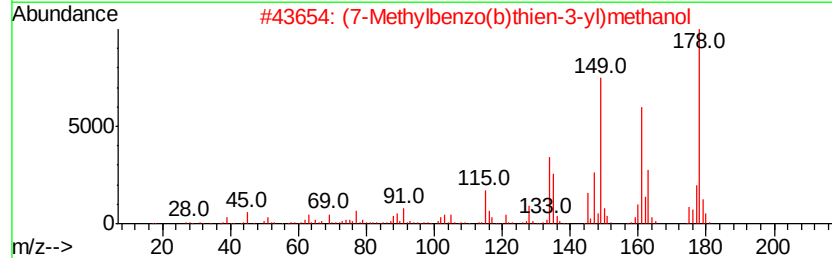
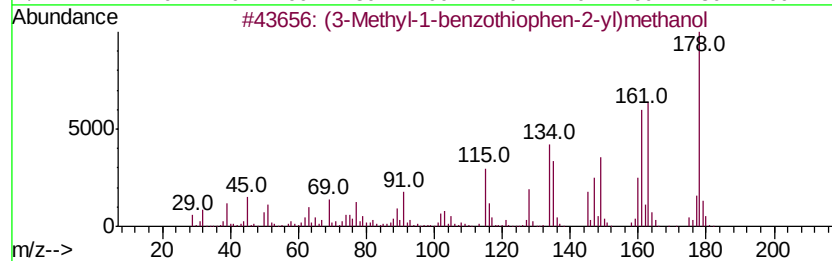
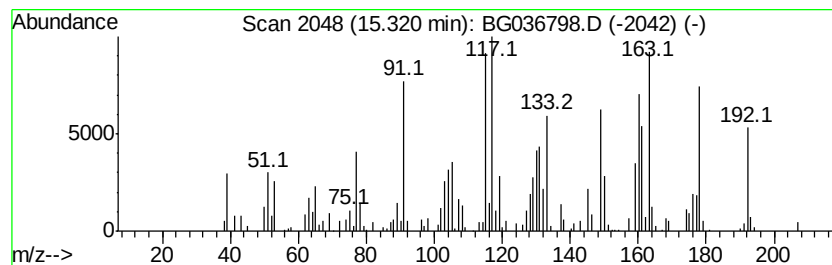
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.32 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.32	4.98 ng	180491	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Methyl-1-benzothiophen-2-yl)m...	178	C10H100S	003133-88-8	22
2	(7-Methylbenzo(b)thien-3-yl)meth...	178	C10H100S	007354-45-2	22
3	4-Amino-2-nitrobenzonitrile	163	C7H5N3O2	072115-07-2	18
4	1-(5-Dimethylethyl)pyrazin-2-yl-...	178	C10H14N2O	182306-61-2	14
5	1,4-Benzenediamine, N4-,N4-dieth...	178	C11H18N2	000148-71-0	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
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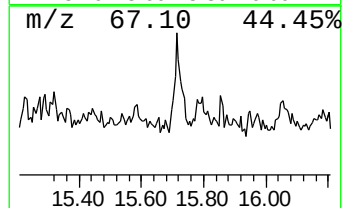
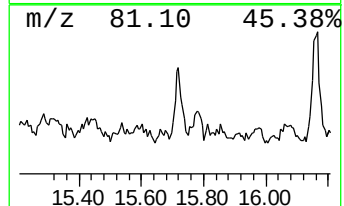
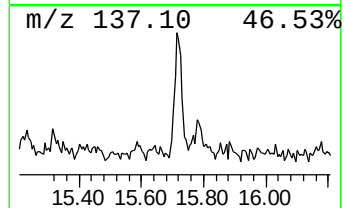
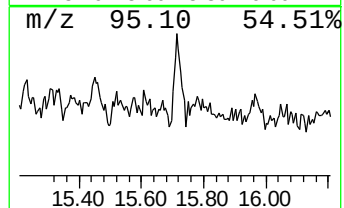
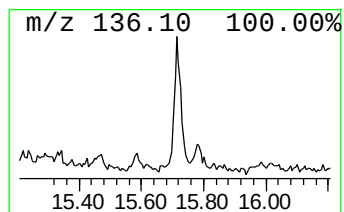
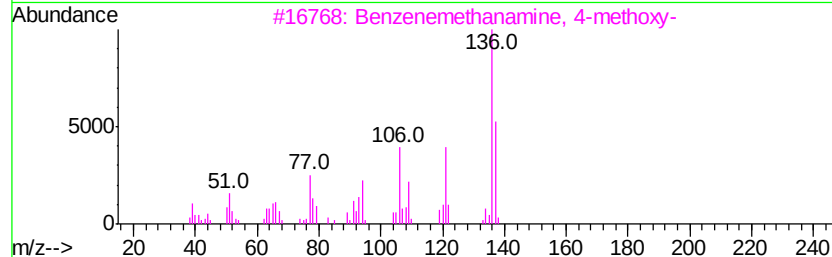
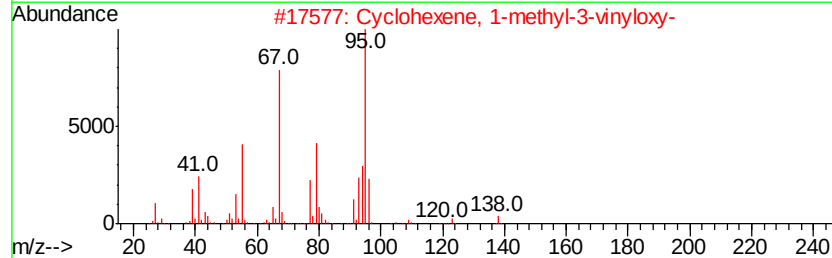
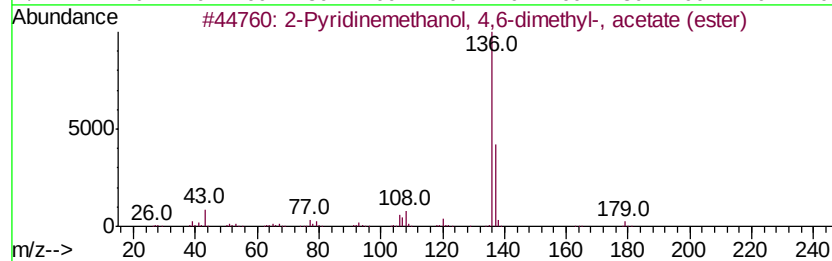
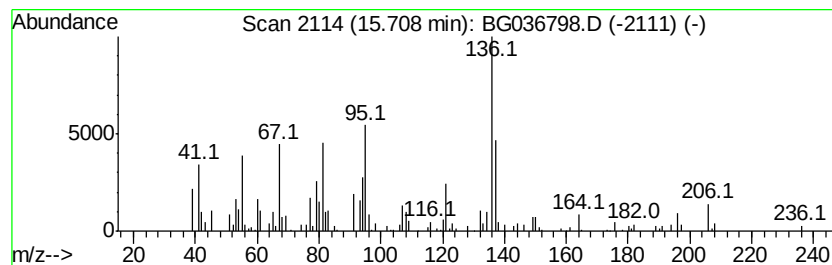
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.71 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.01 ng	108887	Acenaphthene-d10	14.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pyridinemethanol, 4,6-dimethyl...	179	C10H13NO2	020609-14-7	35
2			Cyclohexene, 1-methyl-3-vinyloxy-	138	C9H14O	100144-30-7	35
3			Benzenemethanamine, 4-methoxy-	137	C8H11NO	002393-23-9	35
4			Naphthalene-D8	136	C10D8	001146-65-2	22
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
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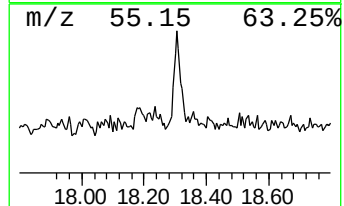
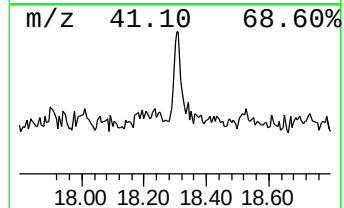
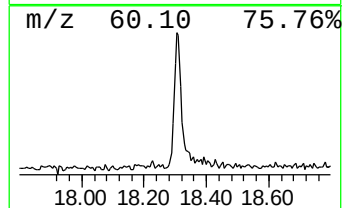
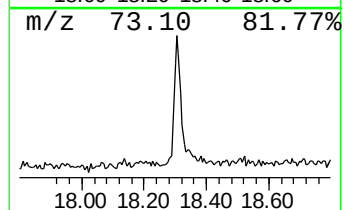
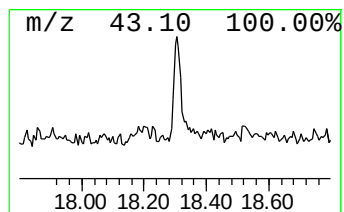
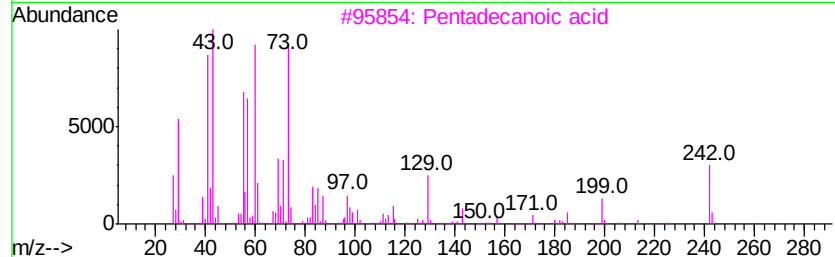
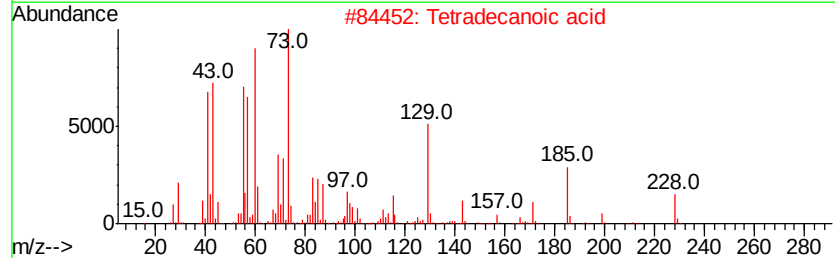
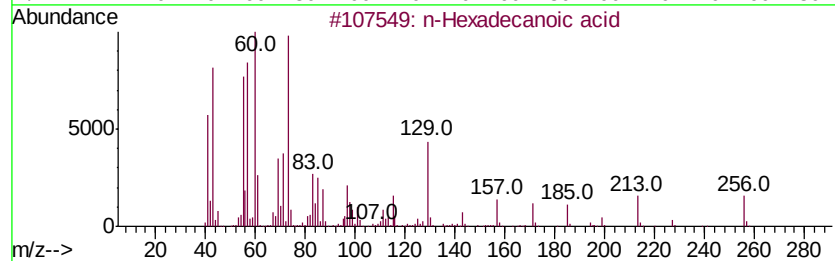
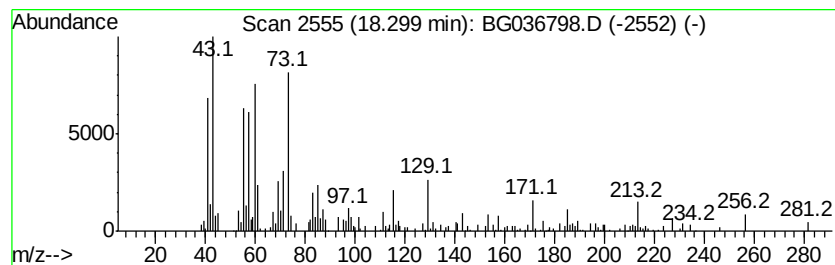
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.07 ng	141437	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Dodecanoic acid	200	C12H24O2	000143-07-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036798.D
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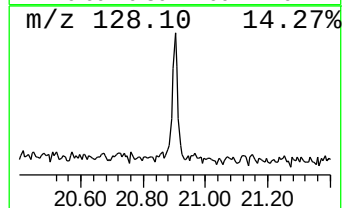
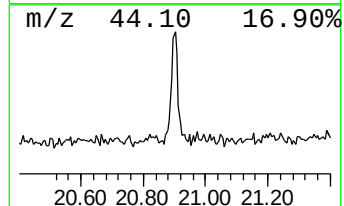
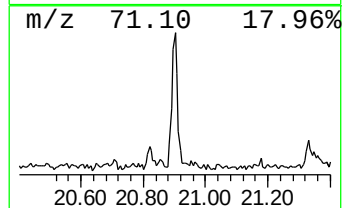
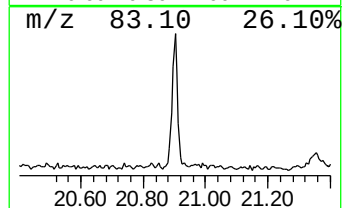
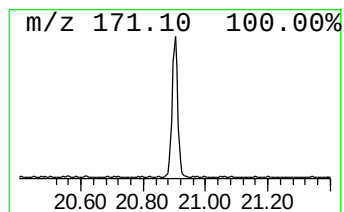
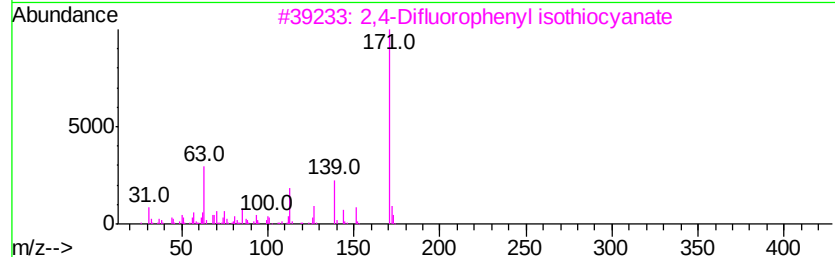
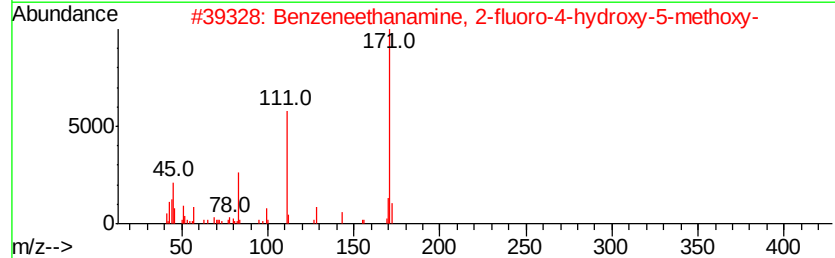
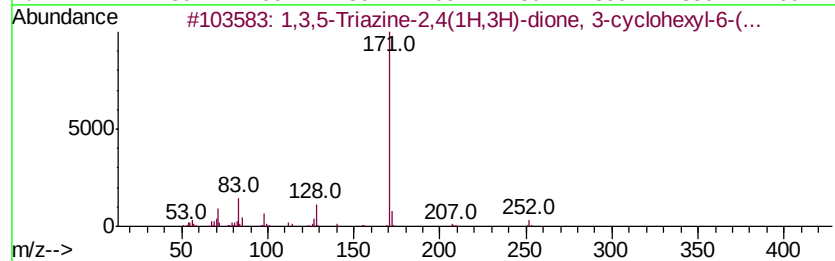
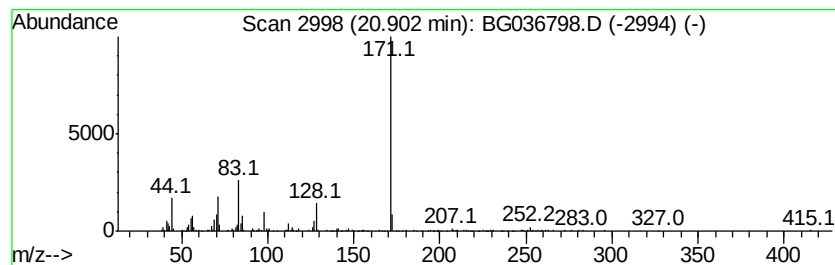
Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.90	3.34 ng	177736	Chrysene-d12	21.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	97
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	72
3	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	50
4	2,6-Difluorophenyl isocyanate	171	C7H3F2NS	065295-69-4	50
5	N-Methoxy-2-carbethoxy-2-carbamo...	188	C7H12N2O4	063859-03-0	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091818\
Data File : BG036798.D
Acq On : 18 Sep 2018 23:03
Operator : JU/SJ
Sample : J4922-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
unknown7.58	7.58	84.3	ng	1236910	1	8.05	293636	20.0
unknown11.70	11.70	3.7	ng	86813	2	10.85	468703	20.0
9-Oxabicyclo[3.3....	12.59	2.3	ng	53242	2	10.85	468703	20.0
9-Undecenol, 2,10...	12.79	3.4	ng	124631	3	14.67	724677	20.0
unknown13.19	13.19	2.2	ng	81036	3	14.67	724677	20.0
Benzoic acid, 2,4...	14.31	2.3	ng	81963	3	14.67	724677	20.0
4-Isopropylphenyl...	14.49	3.6	ng	131073	3	14.67	724677	20.0
unknown15.16	15.16	2.3	ng	82454	3	14.67	724677	20.0
unknown15.32	15.32	5.0	ng	180491	3	14.67	724677	20.0
unknown15.71	15.71	3.0	ng	108887	3	14.67	724677	20.0
n-Hexadecanoic acid	18.30	3.1	ng	141437	4	17.42	920230	20.0
1,3,5-Triazine-2,...	20.90	3.3	ng	177736	5	21.68	1065760	20.0