

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
 Data File : BG036951.D
 Acq On : 25 Sep 2018 16:23
 Operator : JU/SJ
 Sample : J5055-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-B

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-BG092018.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	5.150	312	317	325	rBV	36824	62294	2.44%	0.343%
2	5.614	389	396	410	rBV	721028	1288377	50.49%	7.094%
3	7.206	659	667	681	rBV	723604	1460917	57.25%	8.044%
4	7.576	723	730	750	rBV	718669	1361009	53.34%	7.494%
5	8.040	802	809	817	rBV	151835	280993	11.01%	1.547%
6	8.364	856	864	878	rBV	540903	1009978	39.58%	5.561%
7	9.204	998	1007	1027	rBV	440875	919793	36.04%	5.064%
8	10.843	1277	1286	1297	rBV	204212	409791	16.06%	2.256%
9	13.287	1693	1702	1717	rBV	1137693	1973974	77.36%	10.869%
10	13.452	1725	1730	1737	rBV8	13939	28742	1.13%	0.158%
11	14.116	1834	1843	1850	rBV	239708	499370	19.57%	2.750%
12	14.204	1854	1858	1863	rVV5	20518	38474	1.51%	0.212%
13	14.410	1887	1893	1898	rBV6	58259	134395	5.27%	0.740%
14	14.498	1903	1908	1914	rVB	128407	205107	8.04%	1.129%
15	14.574	1915	1921	1925	rBV6	38261	76583	3.00%	0.422%
16	14.633	1926	1931	1932	rVV3	68810	96908	3.80%	0.534%
17	14.668	1932	1937	1944	rVB2	334791	617819	24.21%	3.402%
18	15.320	2045	2048	2054	rVB	67372	98881	3.87%	0.544%
19	15.391	2055	2060	2065	rBV5	60404	114411	4.48%	0.630%
20	15.455	2066	2071	2076	rBV2	178872	272365	10.67%	1.500%
21	16.155	2185	2190	2198	rBV	914218	1582988	62.03%	8.716%
22	17.412	2400	2404	2410	rBV	405198	661482	25.92%	3.642%
23	20.021	2843	2848	2855	rVB	1845217	2551801	100.00%	14.050%
24	21.319	3067	3069	3077	rVB2	42797	63356	2.48%	0.349%
25	21.677	3124	3130	3144	rVB	457783	822959	32.25%	4.531%
26	21.865	3159	3162	3168	rVB	28725	41975	1.64%	0.231%
27	22.471	3261	3265	3270	rVB	40318	60399	2.37%	0.333%
28	23.158	3377	3382	3392	rVB2	58007	115975	4.54%	0.639%
29	23.346	3410	3414	3425	rVB	52954	110183	4.32%	0.607%
30	23.957	3513	3518	3525	rVB2	64885	129593	5.08%	0.714%
31	24.885	3666	3676	3690	rVB2	315706	954340	37.40%	5.255%
32	26.025	3862	3870	3878	rVB2	41406	116501	4.57%	0.641%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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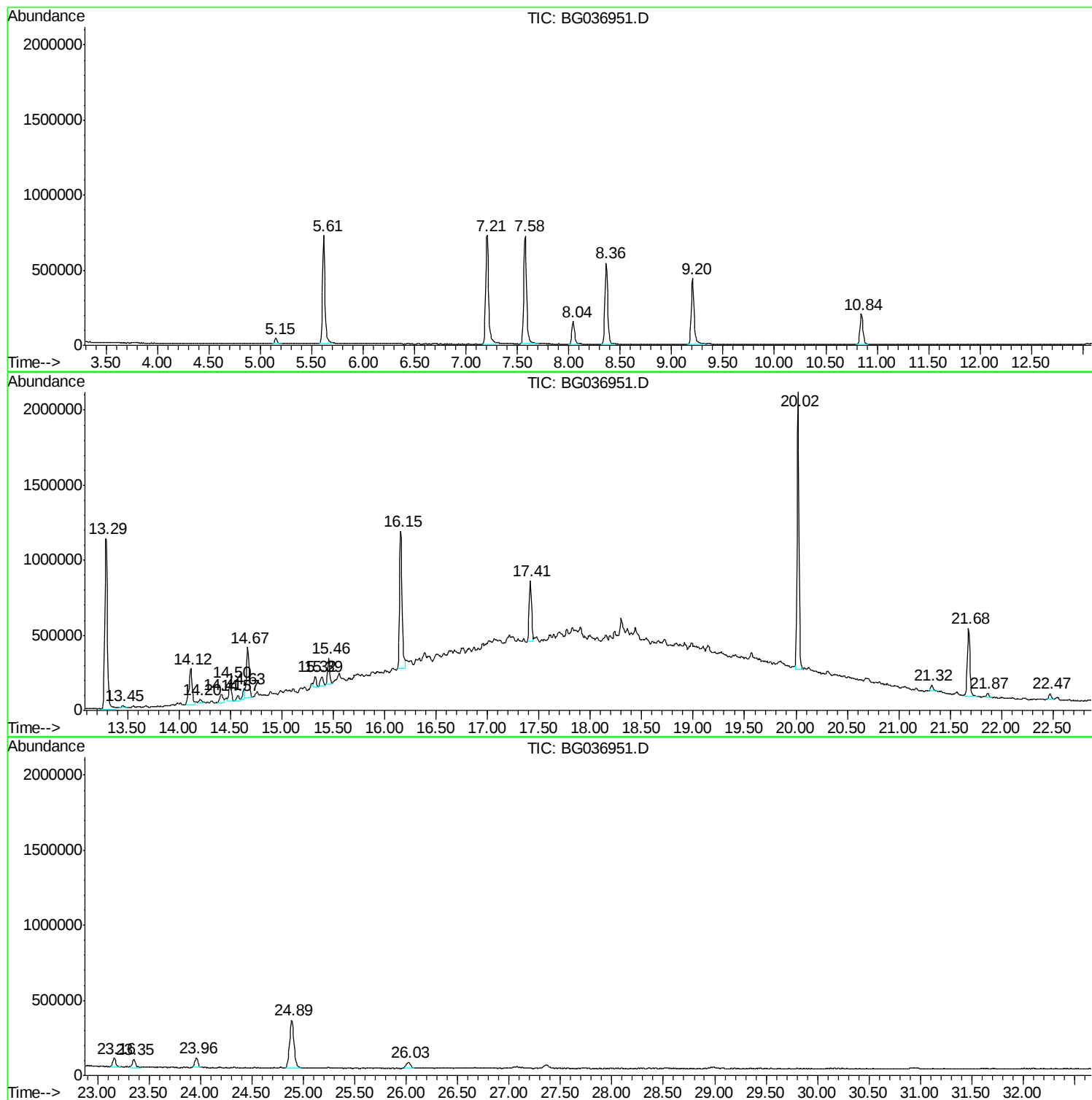
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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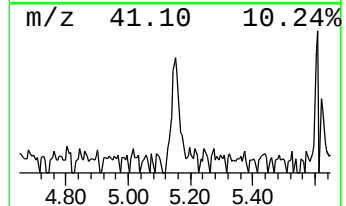
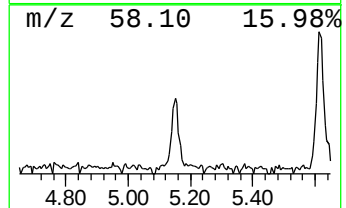
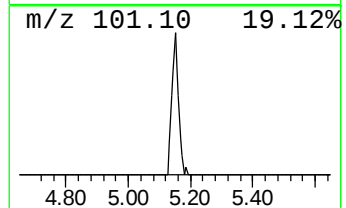
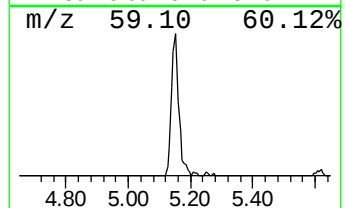
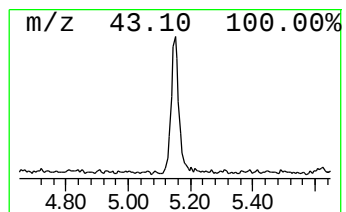
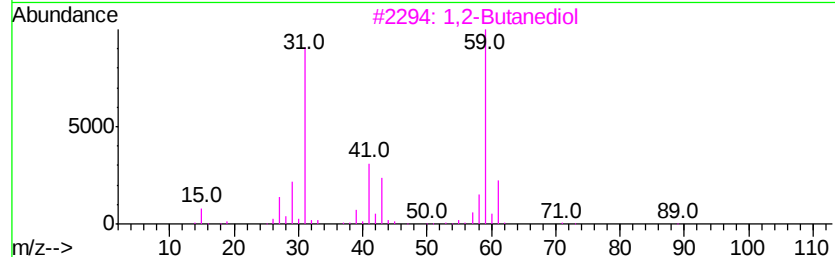
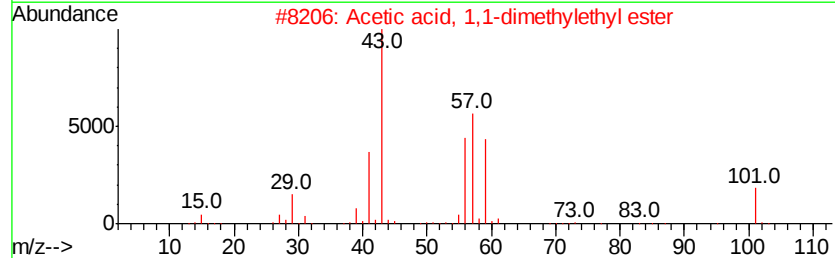
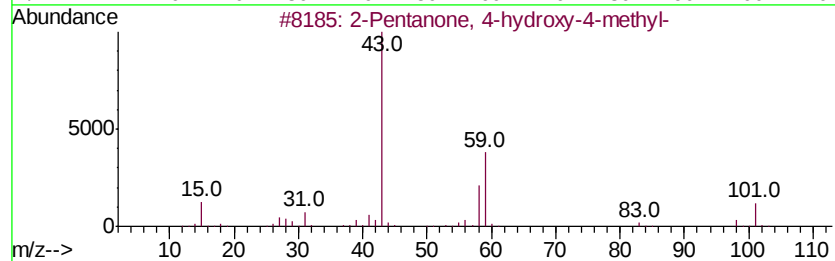
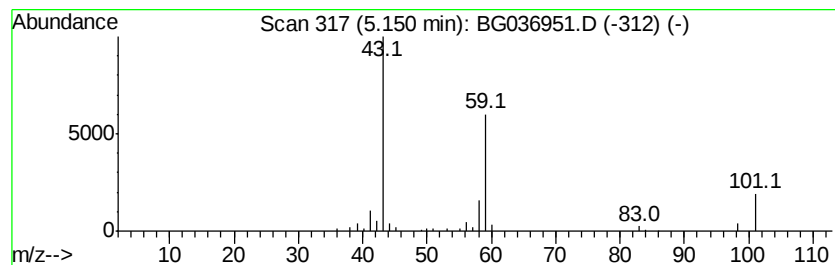
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.43 ng	62294	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		1,2-Butanediol	90	C4H10O2	000584-03-2	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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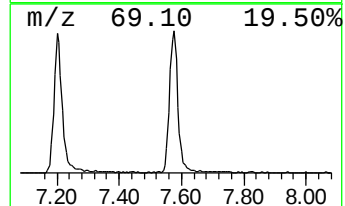
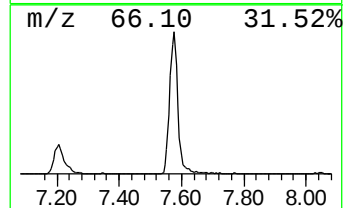
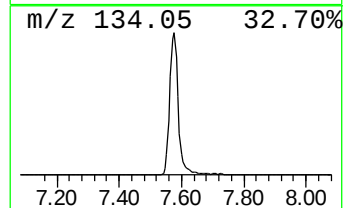
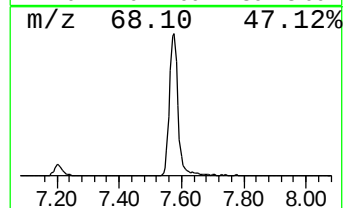
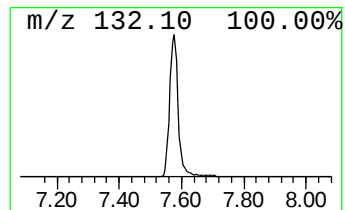
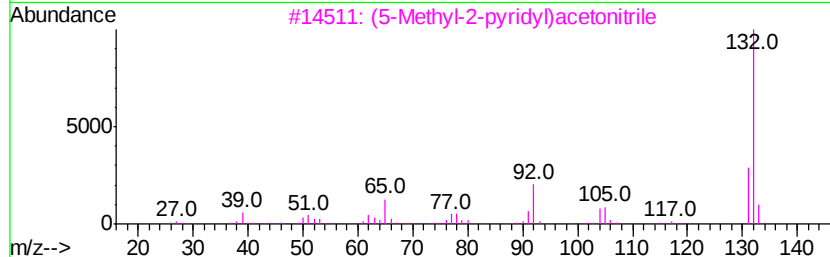
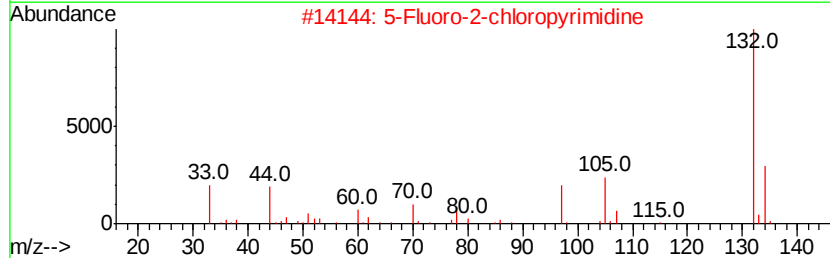
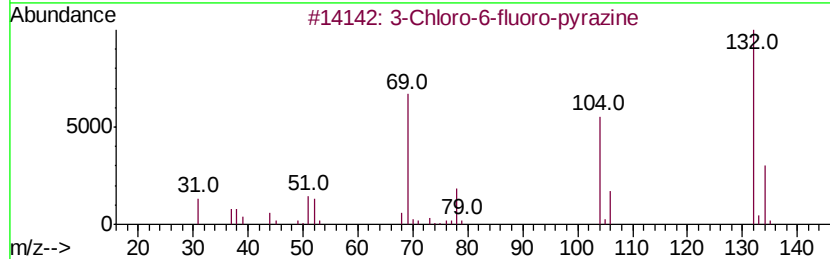
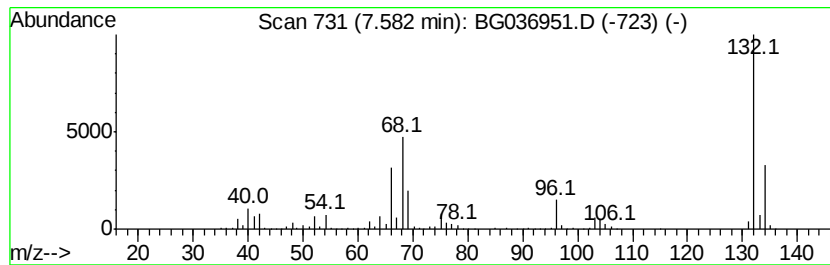
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	96.87 ng	1361010	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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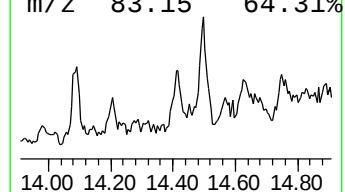
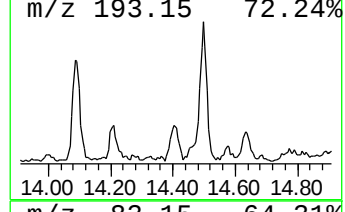
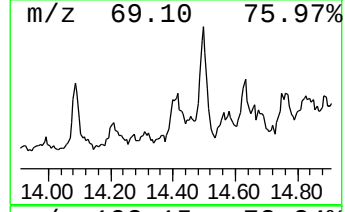
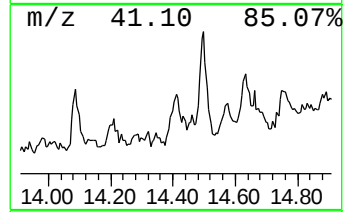
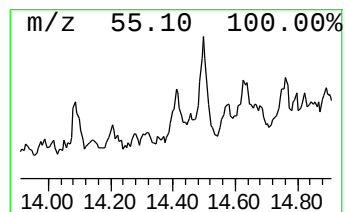
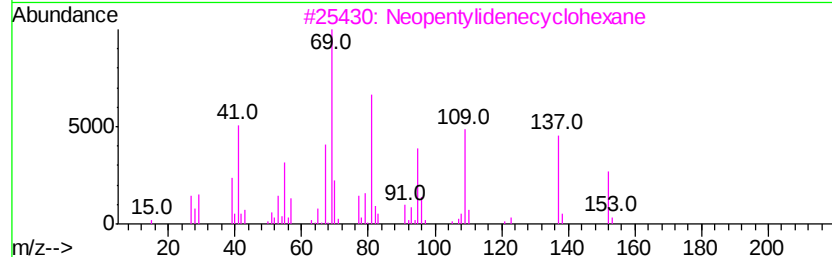
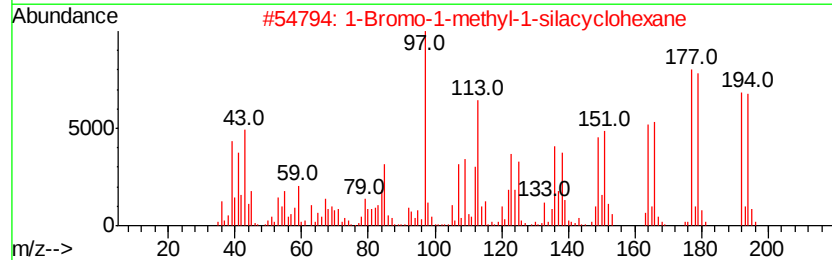
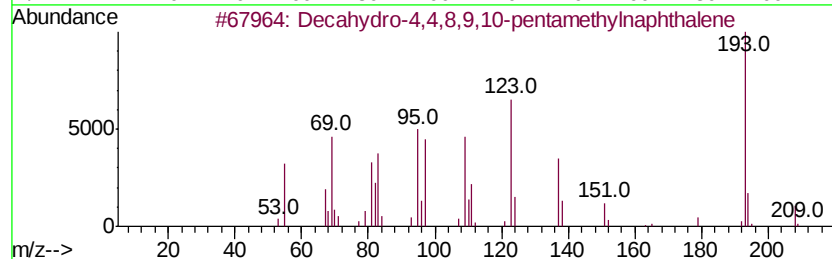
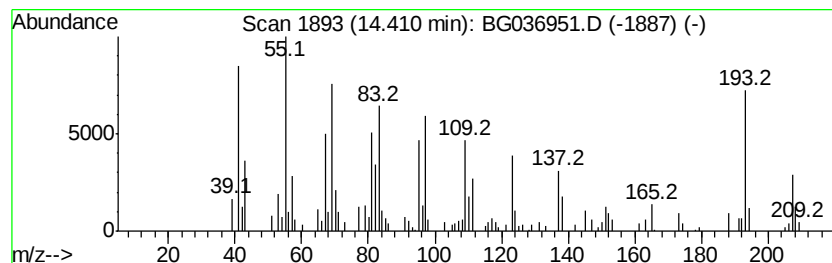
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decahydro-4,4,8,9,10-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	4.35 ng	134395	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208 C15H28	080655-44-3 92
2		1-Bromo-1-methyl-1-silacyclohexane	192 C6H13BrSi	085125-32-2 53
3		Neopentylidenecyclohexane	152 C11H20	039546-80-0 42
4		Succinic acid, di(3,7-dimethylloc...	394 C24H42O4	1000353-35-2 38
5		Cyclohexane, 1-(cyclohexylmethyl...	208 C15H28	054934-92-8 35



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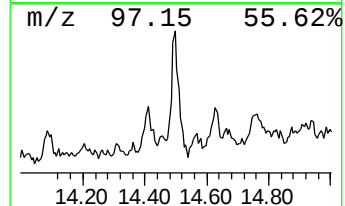
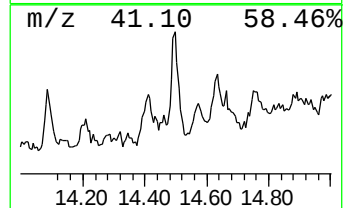
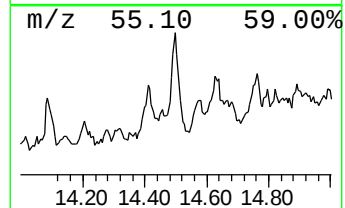
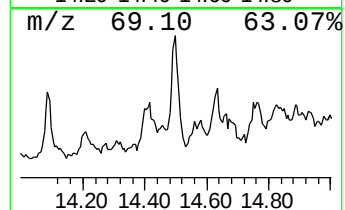
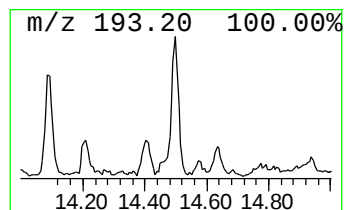
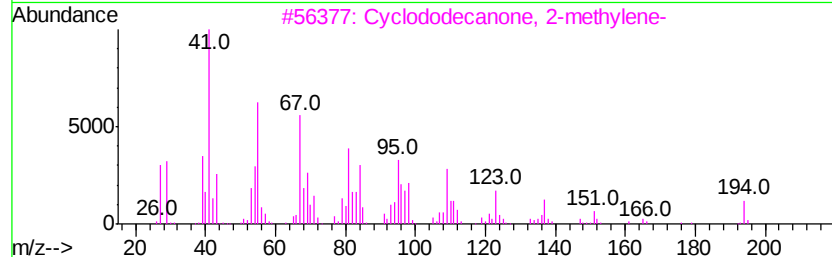
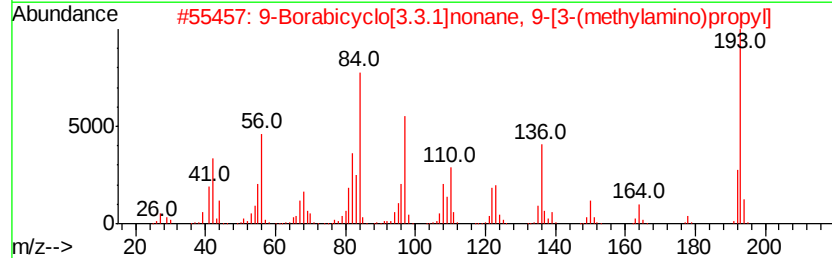
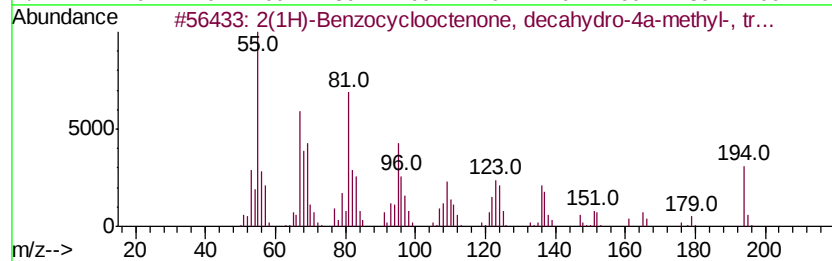
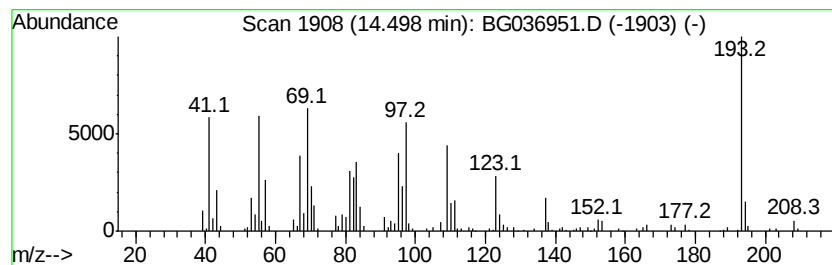
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Peak Number 5 2(1H)-Benzocyclooctenone, d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	6.64 ng	205107	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2(1H)-Benzocyclooctenone, decahy...	194 C13H22O	055103-66-7 50
2		9-Borabicyclo[3.3.1]nonane, 9-[3...	193 C12H24BN	1000162-56-0 47
3		Cyclododecanone, 2-methylene-	194 C13H22O	003045-76-9 43
4		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138 C10H18	004863-59-6 30
5		Iminostilbene	193 C14H11N	000256-96-2 27



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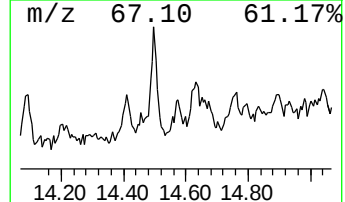
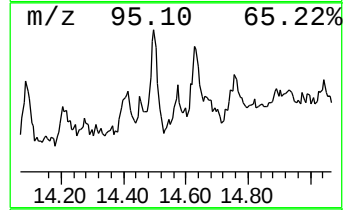
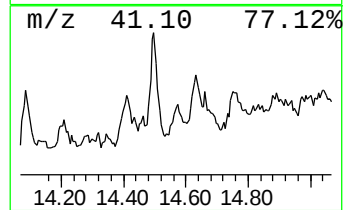
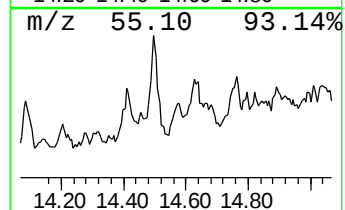
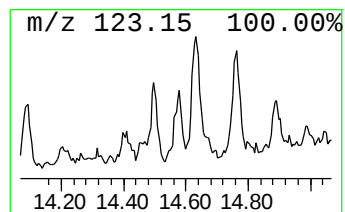
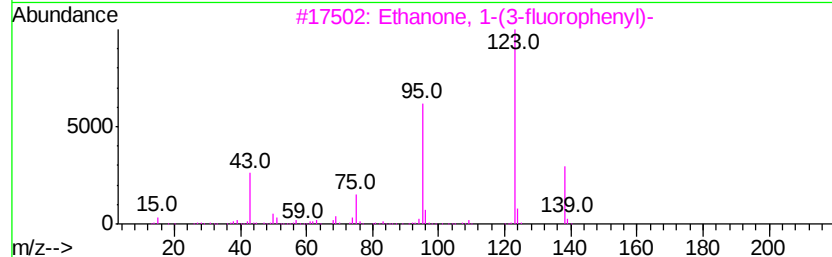
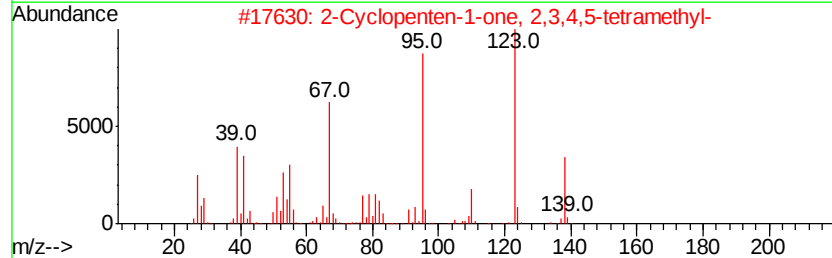
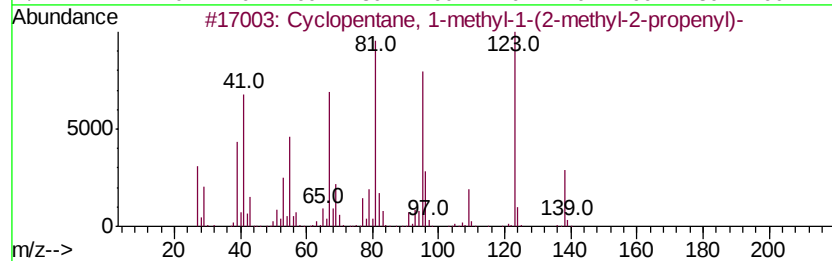
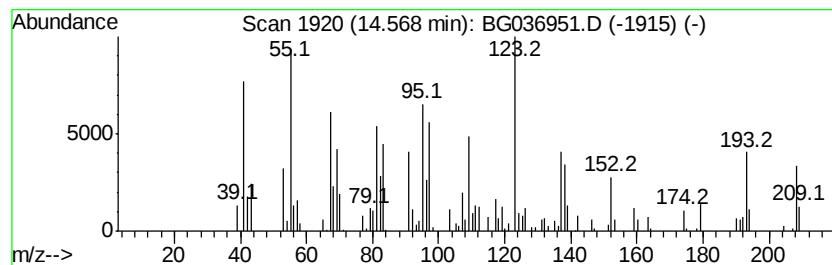
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Peak Number 6 unknown14.57 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.48 ng	76583	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentane, 1-methyl-1-(2-meth...	138 C10H18	074764-47-9 49
2		2-Cyclopenten-1-one, 2,3,4,5-tet...	138 C9H14O	054458-61-6 43
3		Ethanone, 1-(3-fluorophenyl)-	138 C8H7FO	000455-36-7 43
4		Ethanone, 1-(4-fluorophenyl)-	138 C8H7FO	000403-42-9 38
5		3-Fluoropropiophenone	152 C9H9FO	000455-67-4 38



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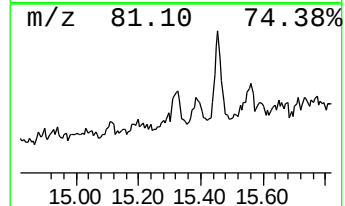
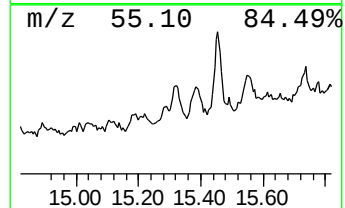
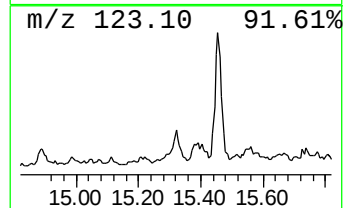
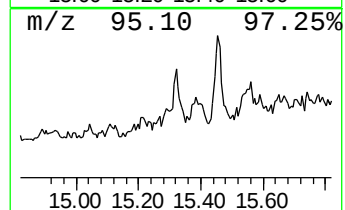
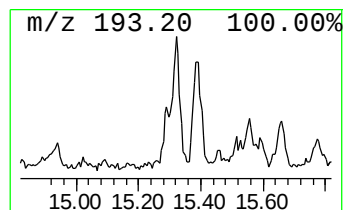
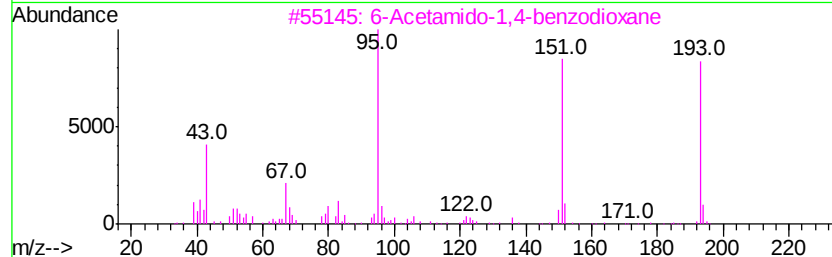
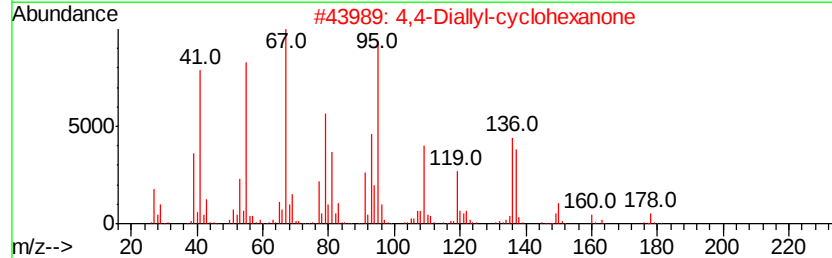
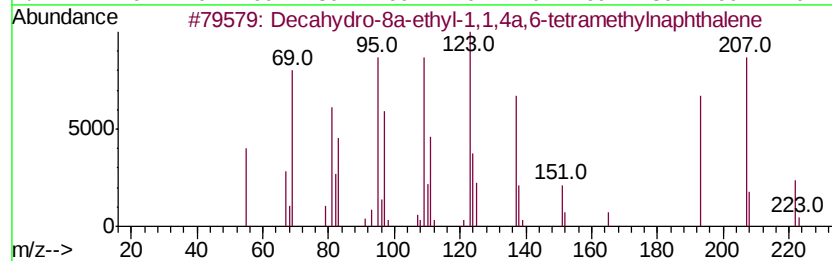
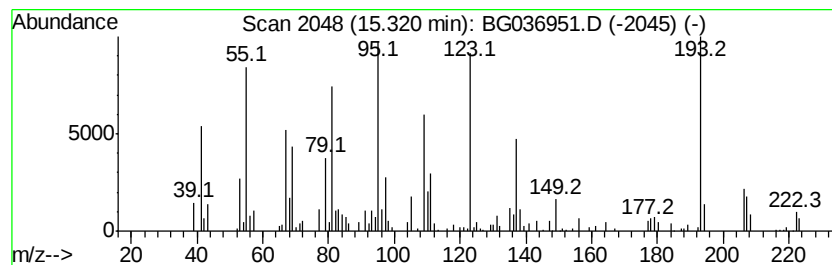
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.32 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.32	3.20 ng	98881	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	46
2	4,4-Diallyl-cyclohexanone	178	C12H18O	1000186-50-2	30
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	30
4	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	25
5	Cyclohexanecarboxamide, N-furfuryl-	207	C12H17NO2	006341-32-8	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
Data File : BG036951.D
Acq On : 25 Sep 2018 16:23
Operator : JU/SJ
Sample : J5055-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

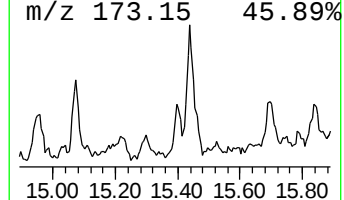
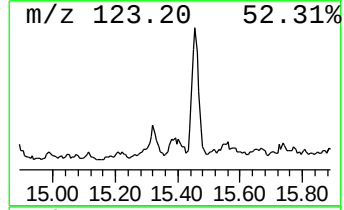
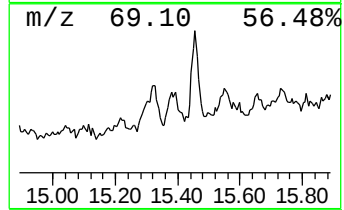
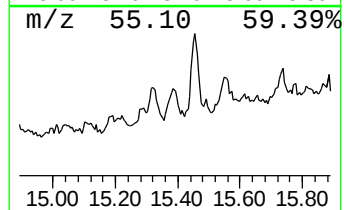
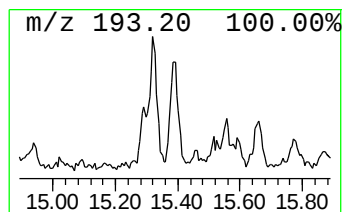
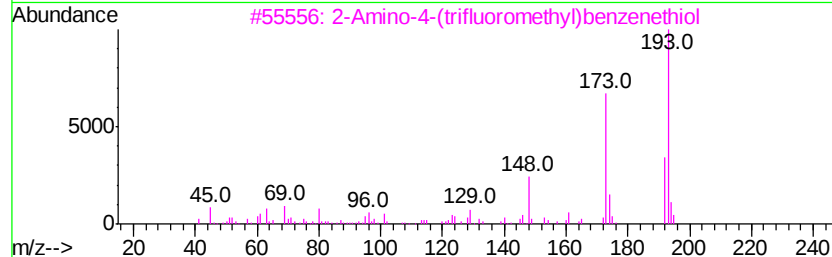
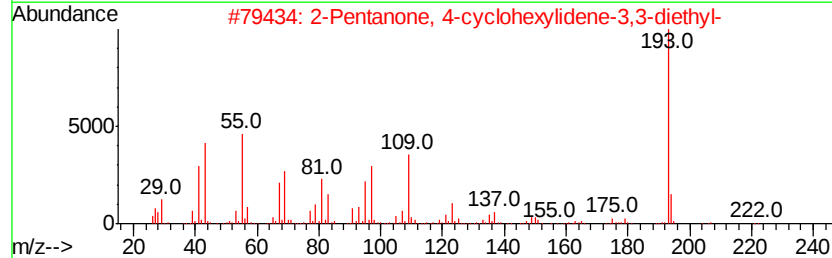
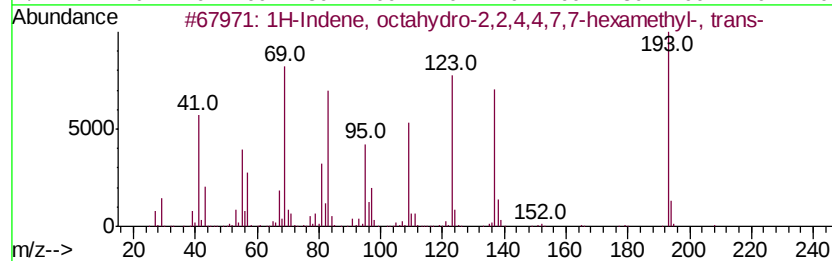
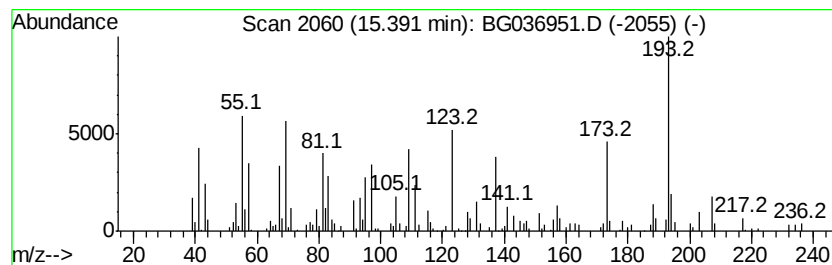
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.39 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.39	3.70 ng	114411	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3	2-Amino-4-(trifluoromethyl)benze...	193	C7H6F3NS	004274-38-8	27
4	Acetophenone, 2'-(trimethylsiloxy)-	208	C11H16O2Si	033342-85-7	14
5	3-Aminophenanthrene	193	C14H11N	001892-54-2	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
Data File : BG036951.D
Acq On : 25 Sep 2018 16:23
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Sample : J5055-08
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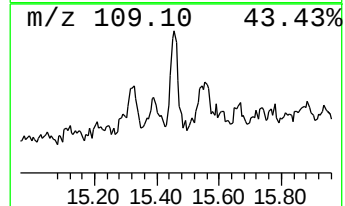
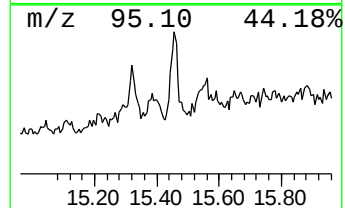
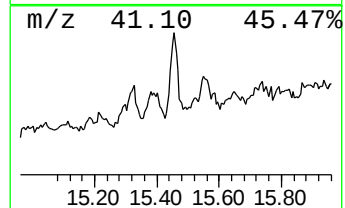
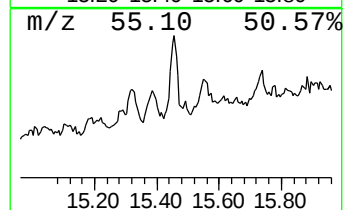
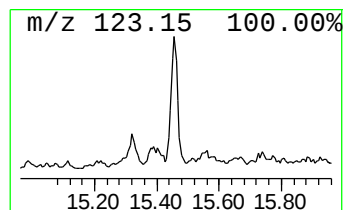
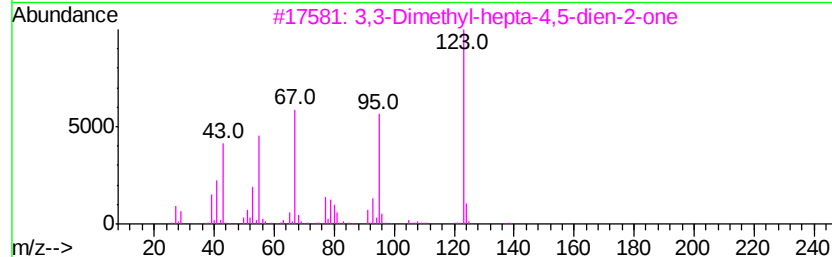
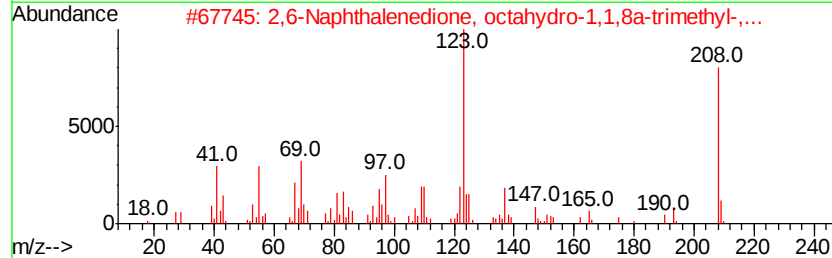
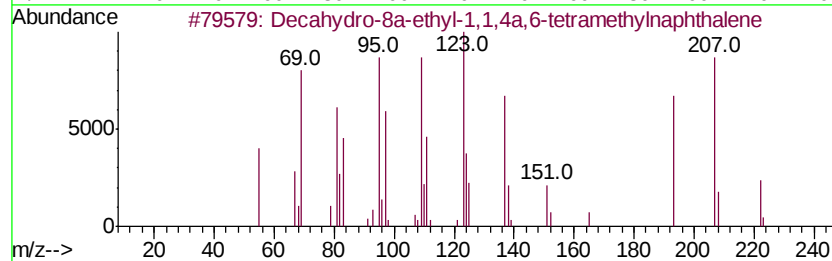
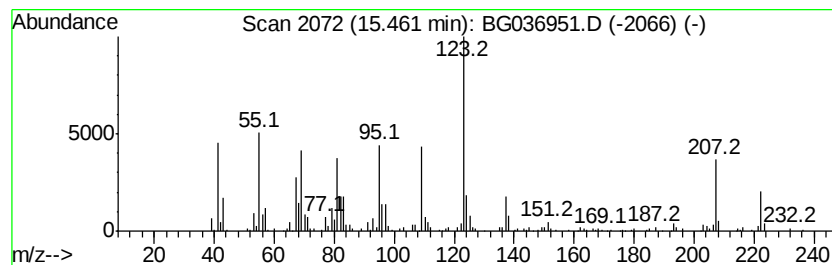
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	8.82 ng	272365	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222 C16H30	1000100-23-6	52
2	2,6-Naphthalenedione, octahydro-...	208 C13H20O2	057289-16-4	47
3	3,3-Dimethyl-hepta-4,5-dien-2-one	138 C9H14O	1000190-54-1	43
4	1,3-Benzenediamine, 4-methoxy-	138 C7H10N2O	000615-05-4	43
5	Magnesium, bis(acetylacetonate)	222 C10H14MgO4	068488-07-3	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
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Sample : J5055-08
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ClientSampleId :
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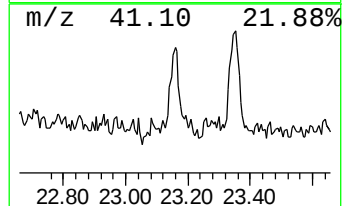
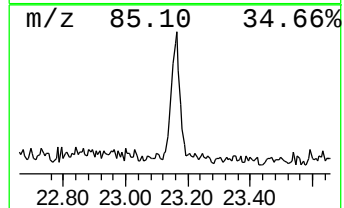
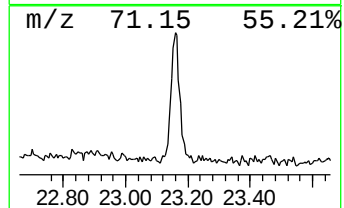
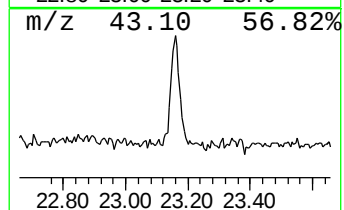
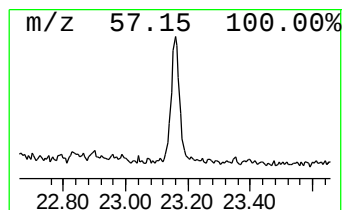
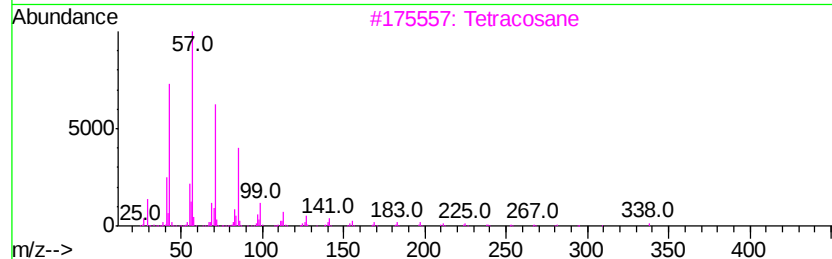
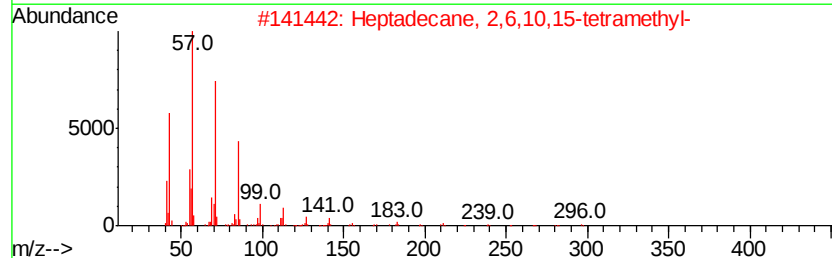
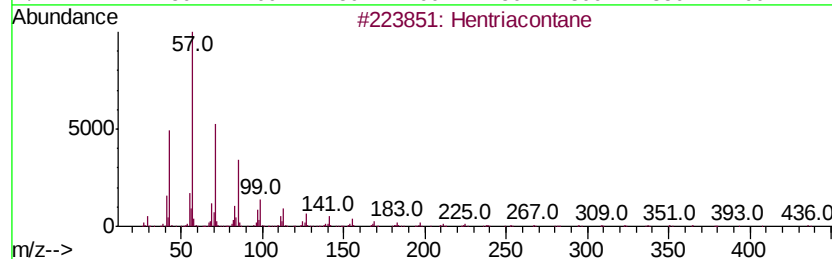
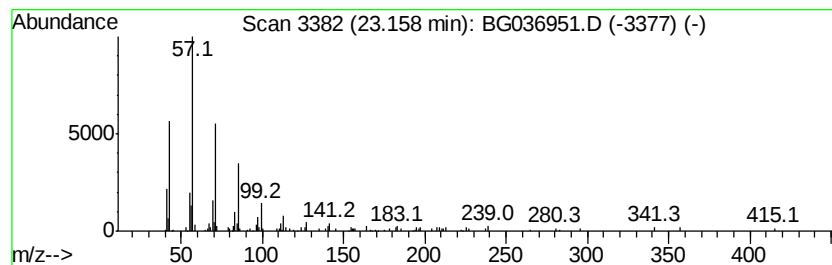
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	2.82 ng	115975	Chrysene-d12	21.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	83
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	80
3	Tetracosane		338	C24H50	000646-31-1	80
4	Tricosane, 2-methyl-		338	C24H50	001928-30-9	80
5	Octadecane		254	C18H38	000593-45-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
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ClientSampleId :
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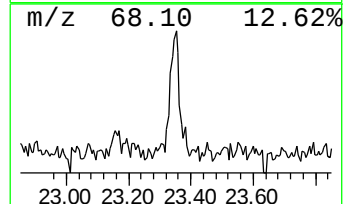
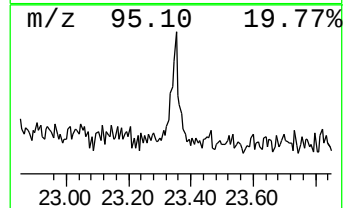
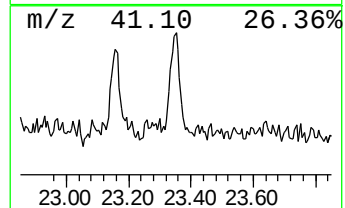
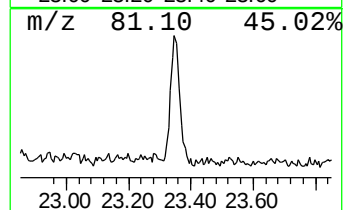
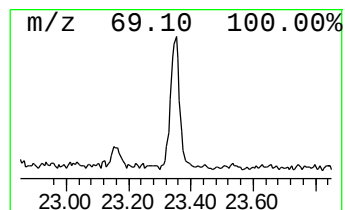
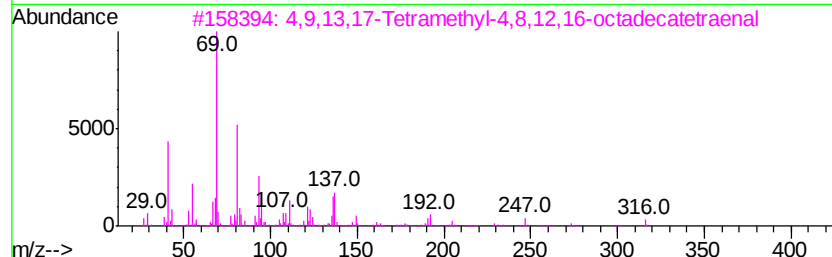
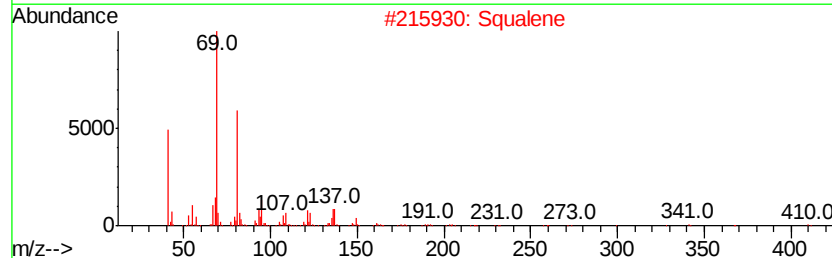
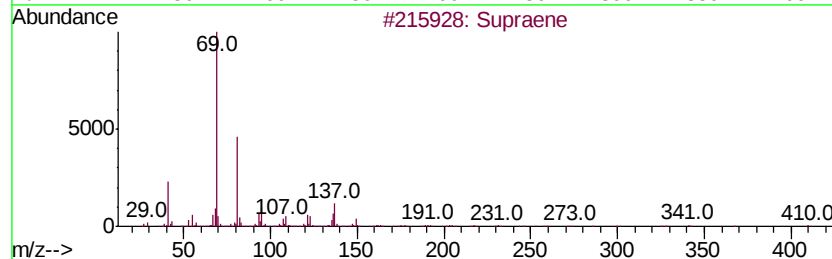
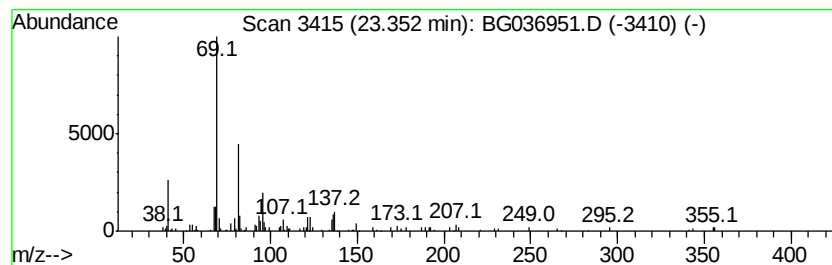
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Supraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.31 ng	110183	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	87
2		Squalene	410	C30H50	000111-02-4	86
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	86
4		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



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Data File : BG036951.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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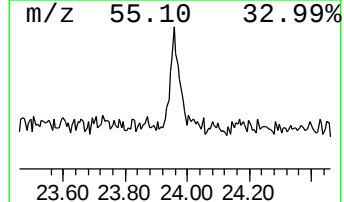
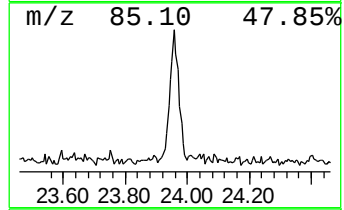
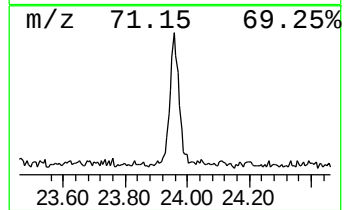
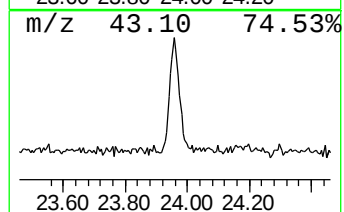
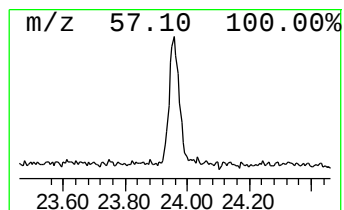
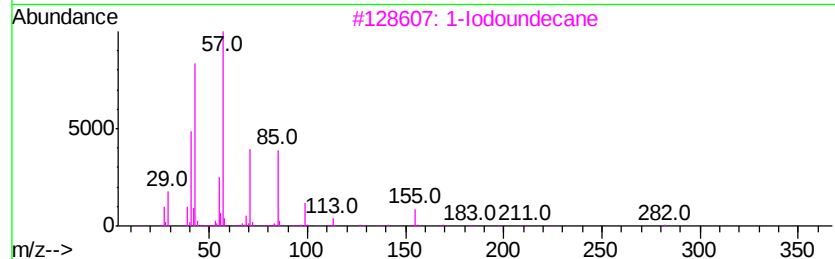
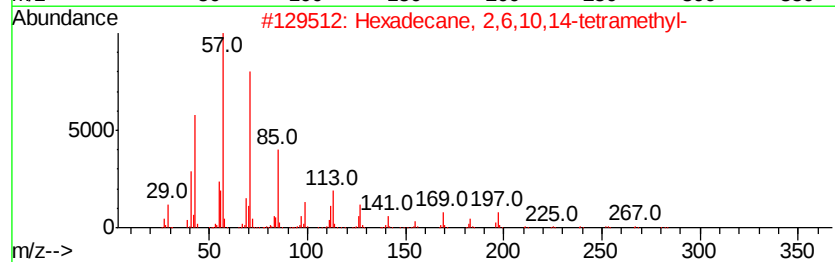
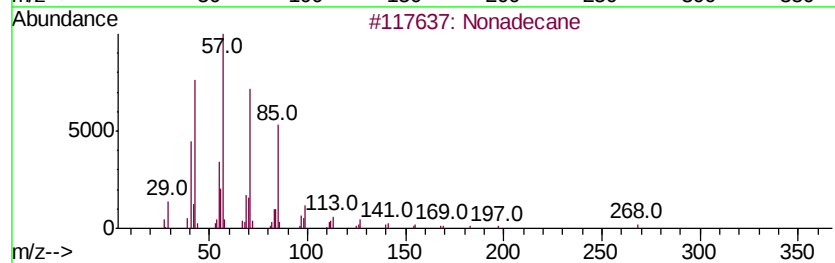
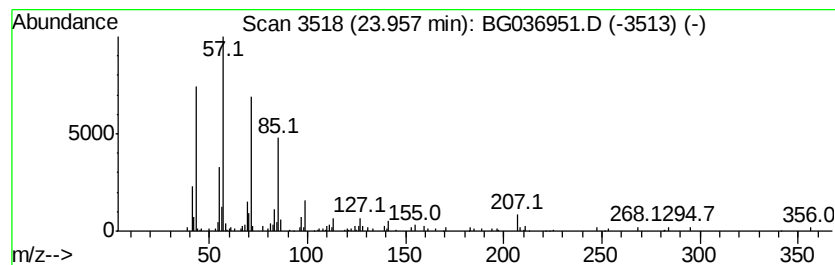
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.96	2.72 ng	129593	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
3		1-Iodoundecane	282	C11H23I	004282-44-4	80
4		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	58
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
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ClientSampleId :
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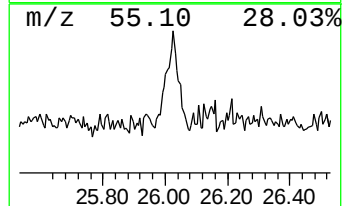
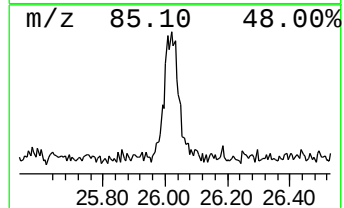
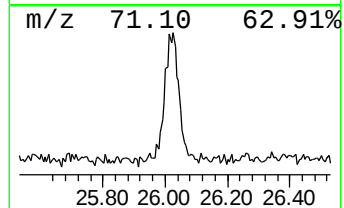
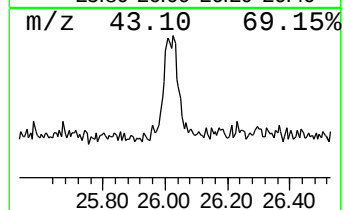
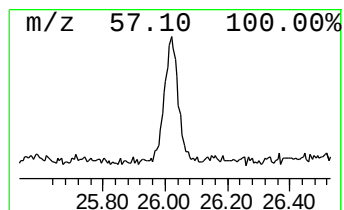
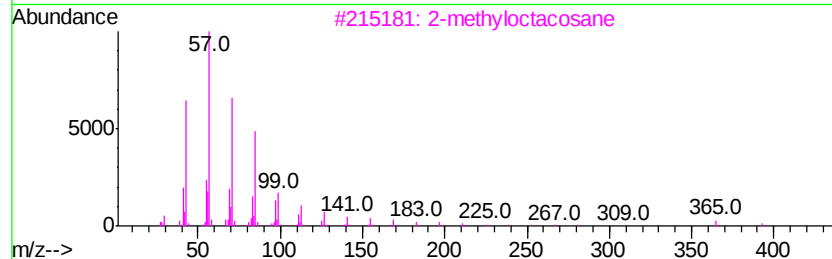
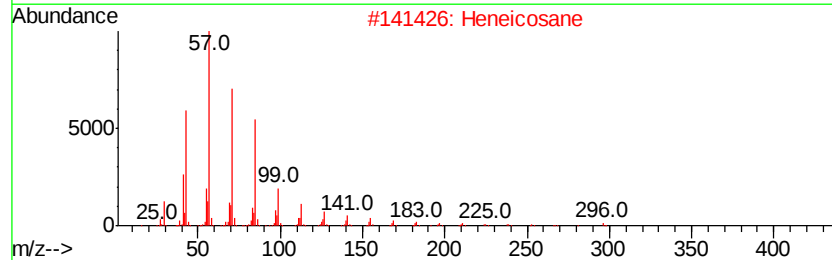
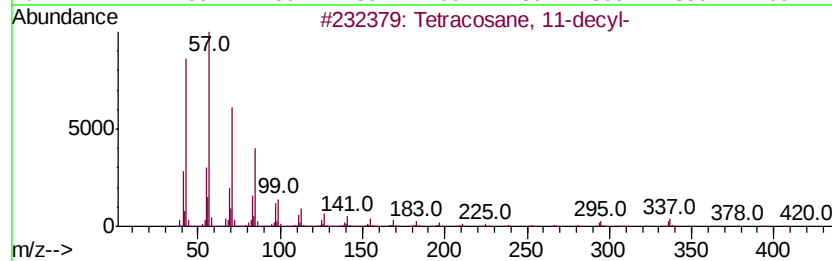
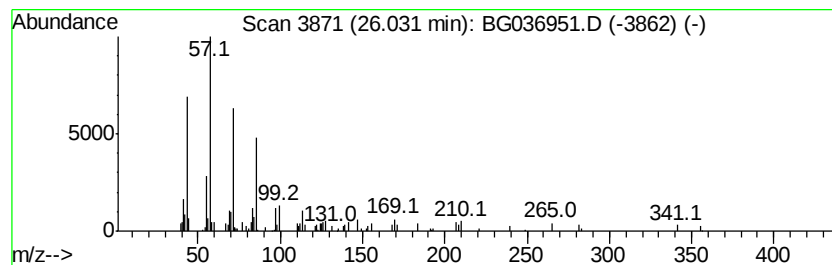
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetracosane, 11-decyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	2.44 ng	116501	Perylene-d12	24.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
2		Heneicosane	296	C21H44	000629-94-7	83
3		2-methyloctacosane	408	C29H60	1000376-72-8	83
4		Tetratetracontane	619	C44H90	007098-22-8	83
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG092518\
Data File : BG036951.D
Acq On : 25 Sep 2018 16:23
Operator : JU/SJ
Sample : J5055-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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
2-Pentanone, 4-hy...	5.15	4.4	ng	62294	1	8.04	280993	20.0
unknown7.58	7.58	96.9	ng	1361010	1	8.04	280993	20.0
Decahydro-4,4,8,9...	14.41	4.3	ng	134395	3	14.67	617819	20.0
2(1H)-Benzocycloo...	14.50	6.6	ng	205107	3	14.67	617819	20.0
unknown14.57	14.57	2.5	ng	76583	3	14.67	617819	20.0
unknown15.32	15.32	3.2	ng	98881	3	14.67	617819	20.0
unknown15.39	15.39	3.7	ng	114411	3	14.67	617819	20.0
Decahydro-8a-ethy...	15.46	8.8	ng	272365	3	14.67	617819	20.0
Hentriacontane	23.16	2.8	ng	115975	5	21.68	822959	20.0
Supraene	23.35	2.3	ng	110183	6	24.89	954340	20.0
Nonadecane	23.96	2.7	ng	129593	6	24.89	954340	20.0
Tetracosane, 11-d...	26.03	2.4	ng	116501	6	24.89	954340	20.0