

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
 Data File : BF084237.D
 Acq On : 4 Jan 2016 14:27
 Operator : UM/SJ
 Sample : G4981-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0531

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:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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	2.167	5	7	17	rVB5	42606	160067	1.60%	0.202%
2	4.259	181	190	192	rVB	31485	112131	1.12%	0.141%
3	5.082	259	262	267	rVB	677431	1083454	10.83%	1.365%
4	5.493	295	298	300	rVB	4095040	3877910	38.78%	4.887%
5	6.522	386	388	390	rBV	3097147	2651961	26.52%	3.342%
6	6.659	397	400	402	rBV	7186518	6728522	67.28%	8.479%
7	6.887	418	420	422	rBV	2485438	2112124	21.12%	2.661%
8	7.047	431	434	436	rBV	7545011	6918099	69.18%	8.717%
9	7.299	452	456	458	rBV	118226	118046	1.18%	0.149%
10	7.459	466	470	472	rBV	6054506	6711560	67.11%	8.457%
11	7.905	507	509	512	rVB	81694	101557	1.02%	0.128%
12	8.179	530	533	535	rBV	2766122	2780496	27.80%	3.504%
13	9.105	609	614	615	rBV2	62802	126390	1.26%	0.159%
14	9.128	615	616	620	rVV2	88422	127817	1.28%	0.161%
15	9.253	624	627	630	rVB	8130064	10000600	100.00%	12.602%
16	9.653	658	662	663	rBV	235089	319511	3.19%	0.403%
17	9.871	678	681	684	rVV	82789	119045	1.19%	0.150%
18	9.928	684	686	688	rVV2	2614757	2871595	28.71%	3.618%
19	9.962	688	689	691	rVB	162387	124846	1.25%	0.157%
20	10.076	697	699	701	rBV	134567	126986	1.27%	0.160%
21	10.259	710	715	721	rBV	132444	736442	7.36%	0.928%
22	10.362	721	724	726	rVV2	161091	330513	3.30%	0.416%
23	10.454	730	732	737	rVB	195340	218984	2.19%	0.276%
24	10.591	741	744	746	rVB	2837076	2854276	28.54%	3.597%
25	10.716	753	755	758	rBV2	4173653	6108491	61.08%	7.697%
26	10.785	758	761	764	rVB	2210682	3349891	33.50%	4.221%
27	10.842	764	766	768	rBV2	128670	174274	1.74%	0.220%
28	11.414	814	816	819	rBV	3031730	2692222	26.92%	3.392%
29	11.631	831	835	837	rBV	569840	601003	6.01%	0.757%
30	12.122	876	878	881	rBV	90447	110175	1.10%	0.139%
31	12.648	922	924	926	rBV	165871	197694	1.98%	0.249%
32	12.785	934	936	938	rBV	499110	489220	4.89%	0.616%
33	12.831	938	940	941	rVV	395862	333576	3.34%	0.420%
34	12.911	944	947	948	rVB2	104961	203189	2.03%	0.256%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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35	13.014	953	956	958	rBV	6791120	8988490	89.88%	11.326%
36	13.117	958	965	967	rVV3	49773	186134	1.86%	0.235%
37	13.540	1000	1002	1003	rBV	171565	190363	1.90%	0.240%
38	13.791	1022	1024	1028	rVB3	194445	278143	2.78%	0.350%
39	13.905	1032	1034	1042	rVB3	204856	513808	5.14%	0.647%
40	14.054	1044	1047	1049	rVB	1822862	1809722	18.10%	2.280%
41	14.225	1060	1062	1069	rVB2	130891	245227	2.45%	0.309%
42	15.494	1170	1173	1175	rBV	1183604	1575051	15.75%	1.985%

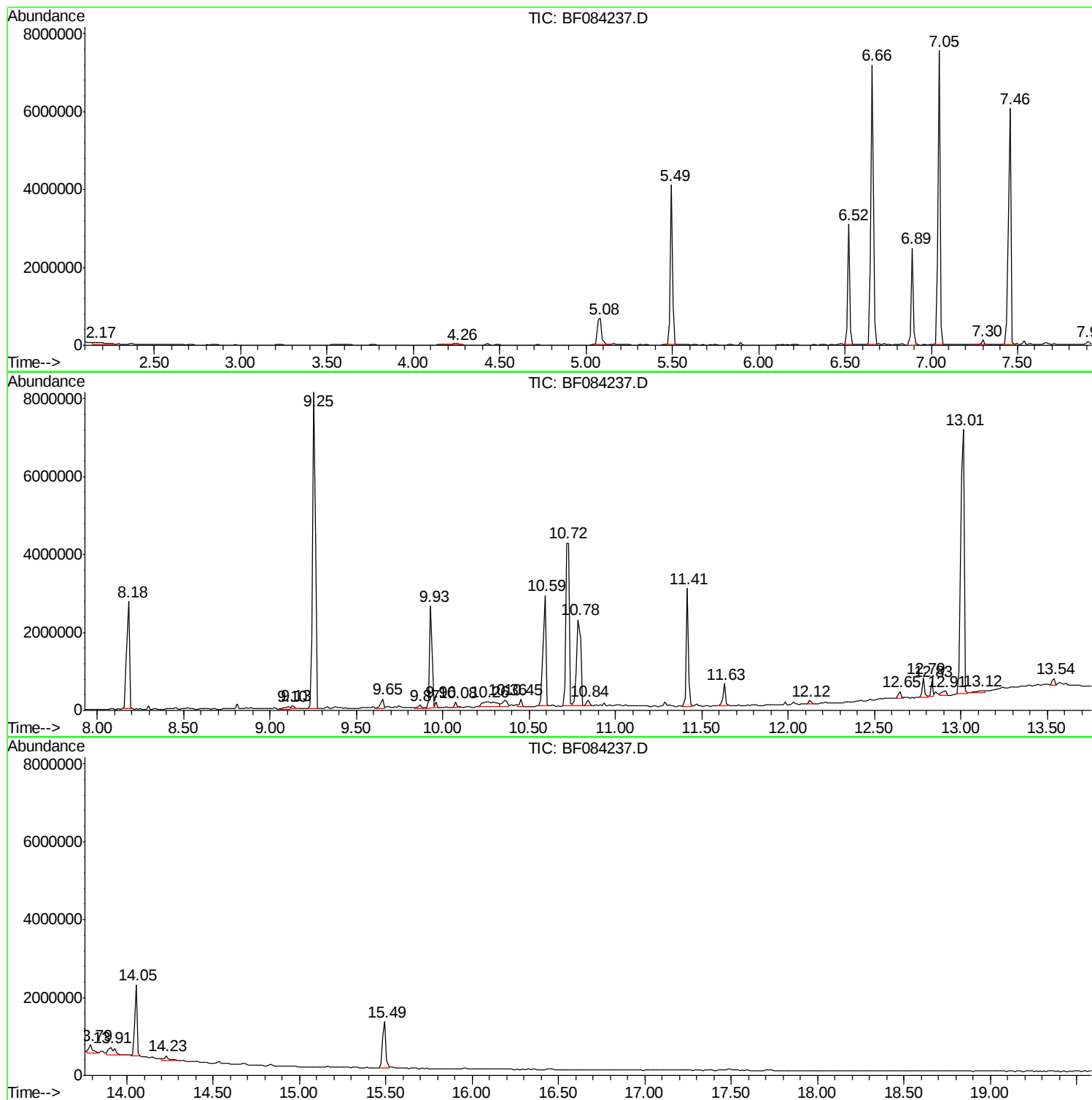
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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S8-0531

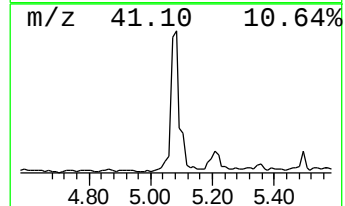
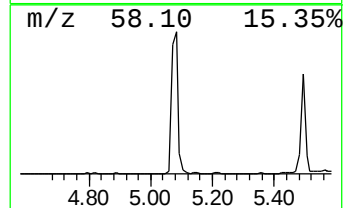
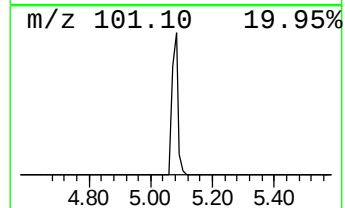
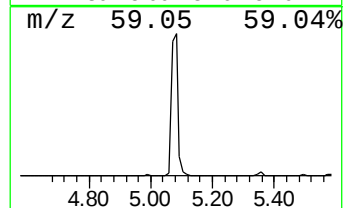
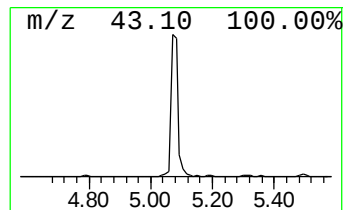
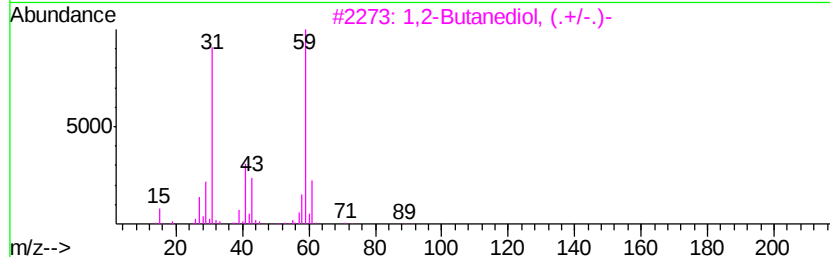
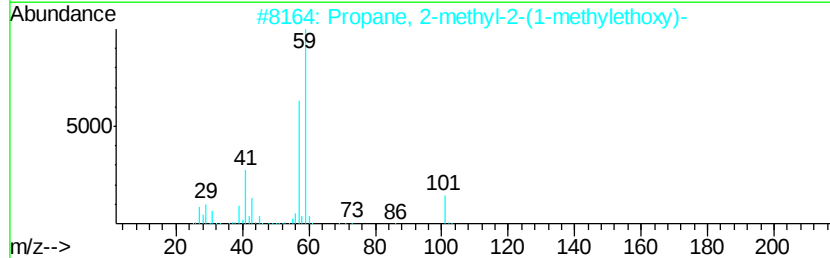
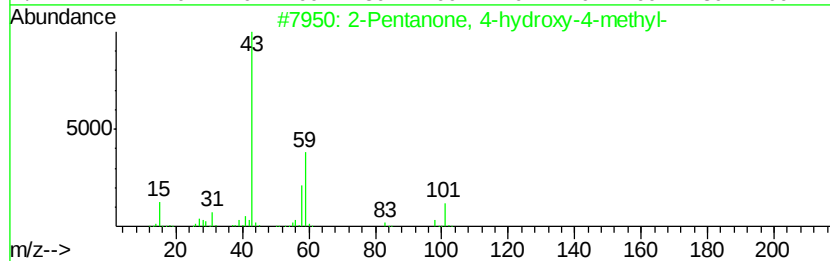
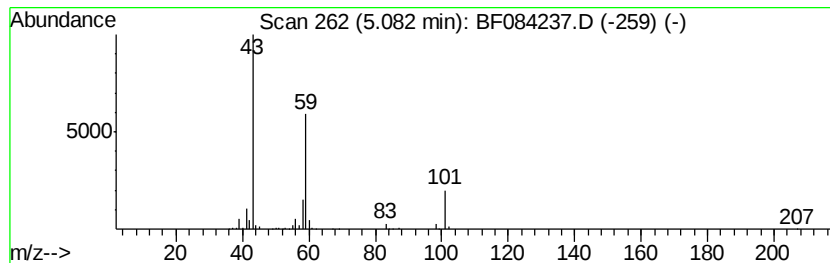
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.08	10.26 ng	1083450	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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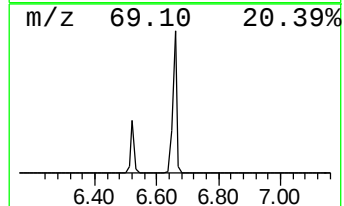
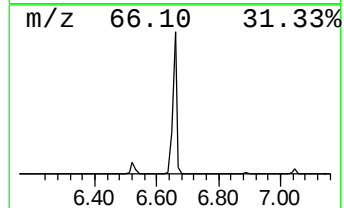
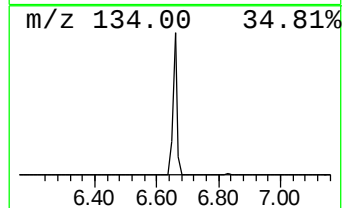
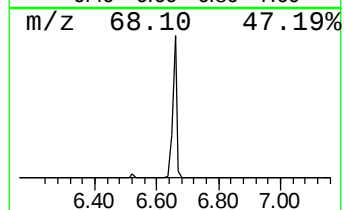
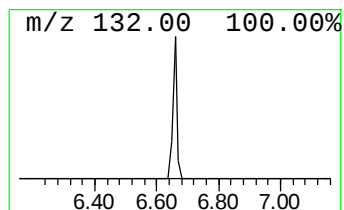
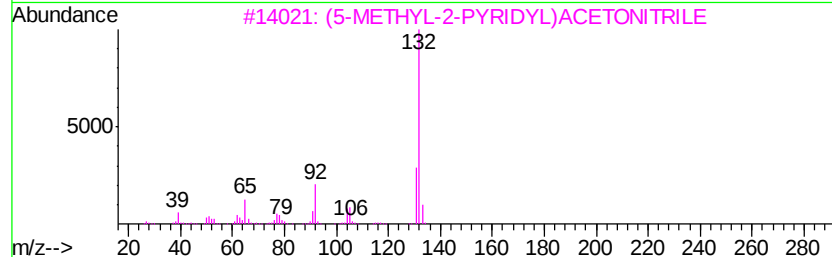
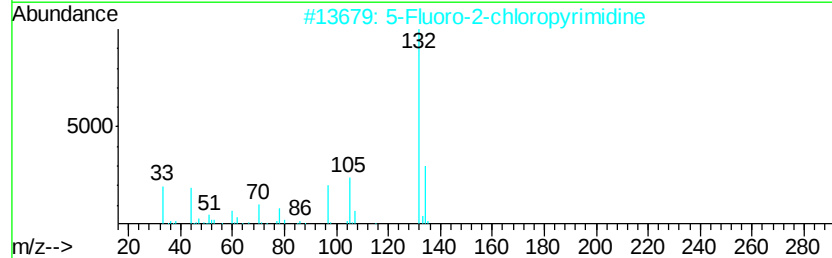
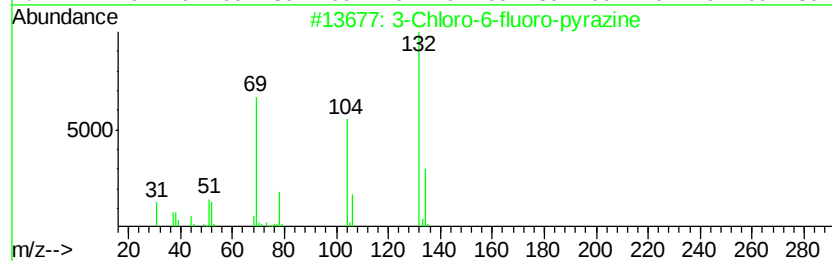
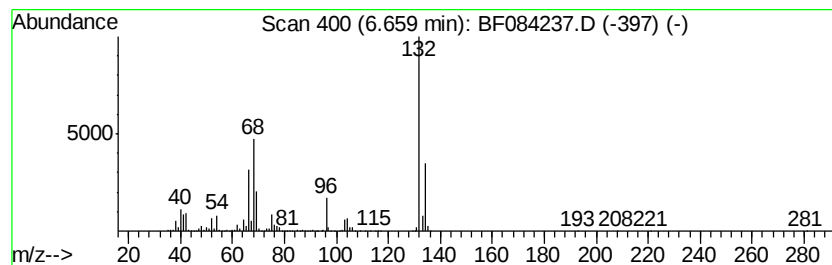
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	63.71 ng	6728520	1,4-Dichlorobenzene-d4	6.89

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		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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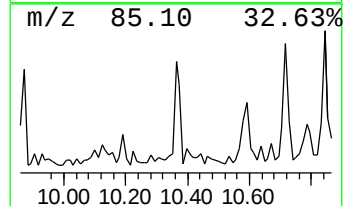
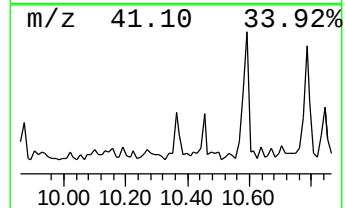
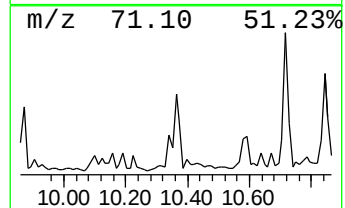
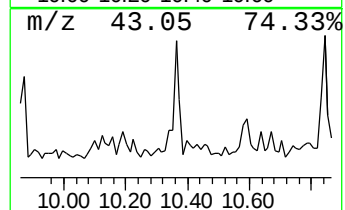
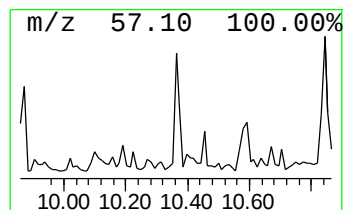
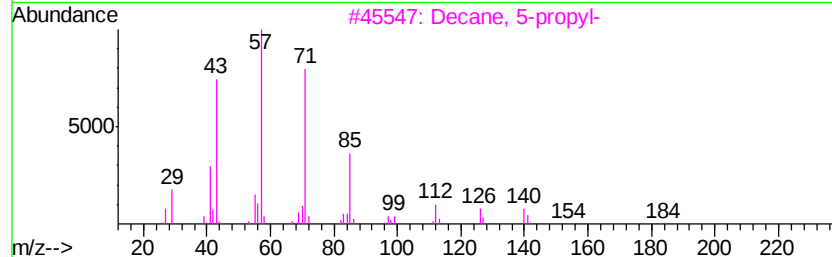
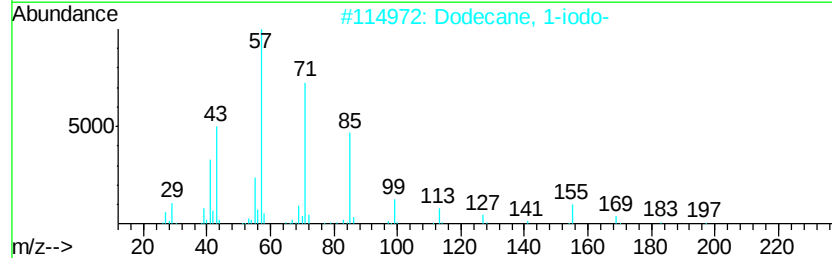
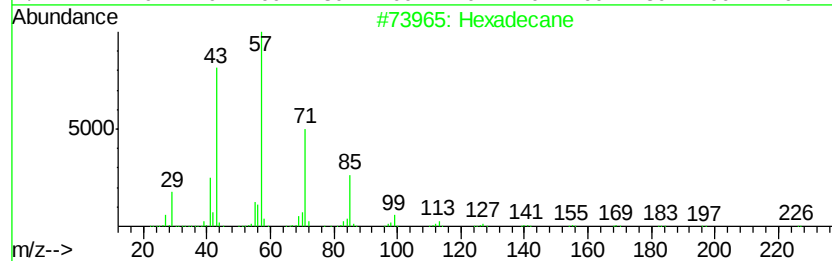
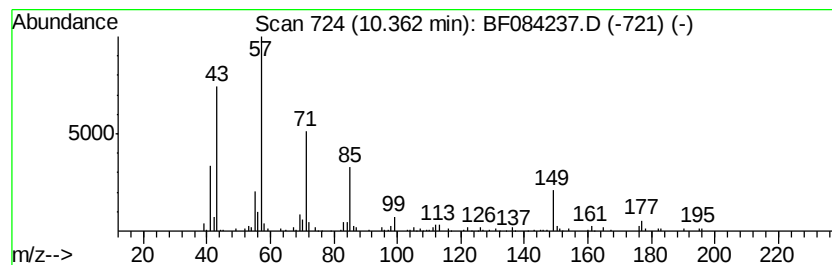
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	2.30 ng	330513	Acenaphthene-d10	9.93
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane		226 C16H34	000544-76-3 72
2	Dodecane, 1-iodo-		296 C12H25I	004292-19-7 59
3	Decane, 5-propyl-		184 C13H28	017312-62-8 59
4	Nonane, 2-methyl-5-propyl-		184 C13H28	031081-17-1 59
5	Tridecane		184 C13H28	000629-50-5 53



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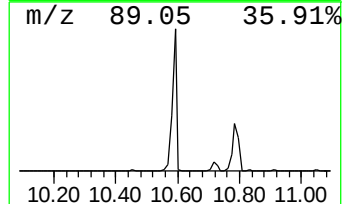
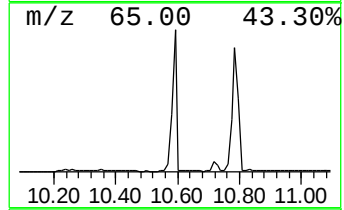
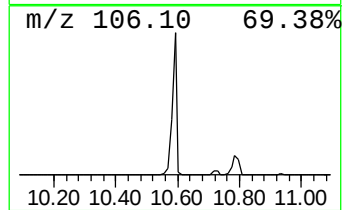
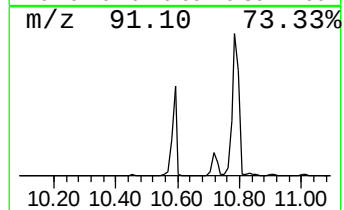
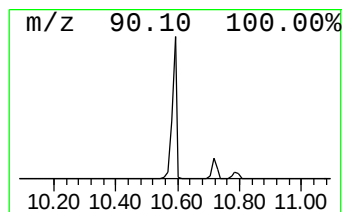
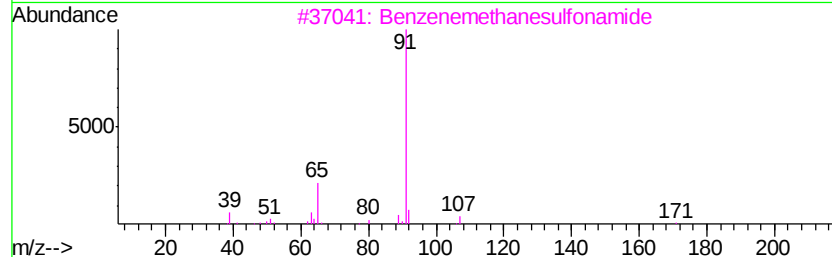
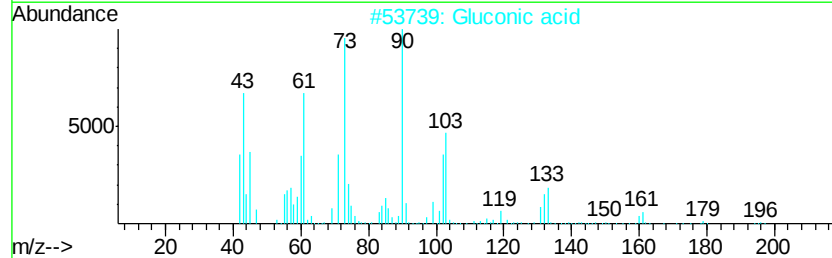
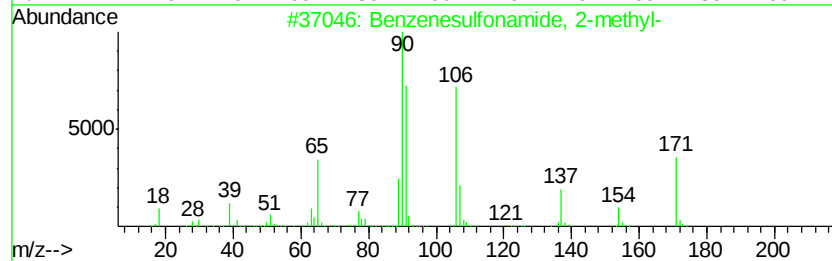
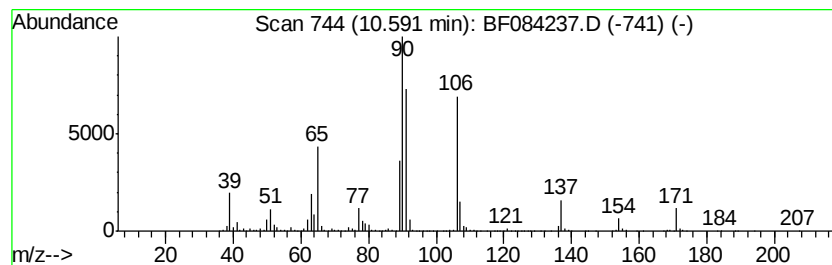
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.59	19.88 ng	2854280	Acenaphthene-d10		9.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2		Gluconic acid	196	C6H12O7	000526-95-4	38
3		Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	30
4		Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	30
5		Thiourea, methyl-	90	C2H6N2S	000598-52-7	25



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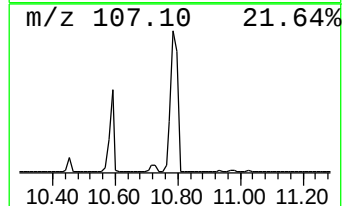
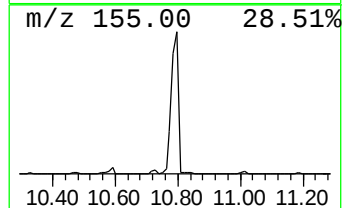
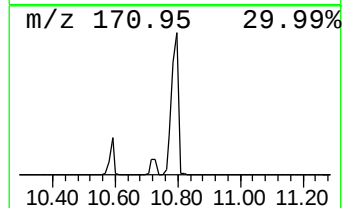
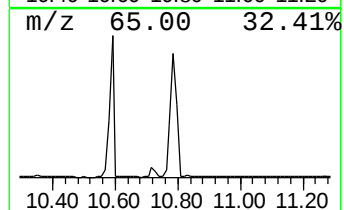
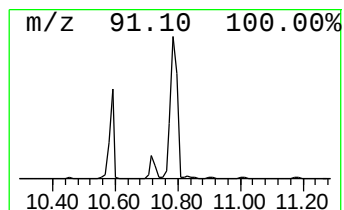
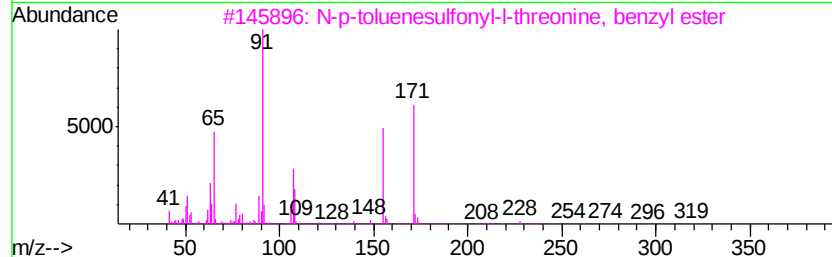
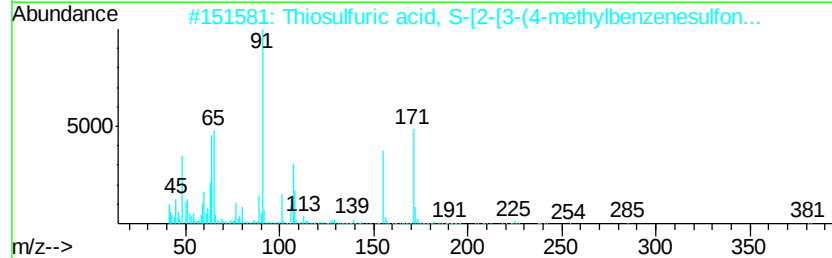
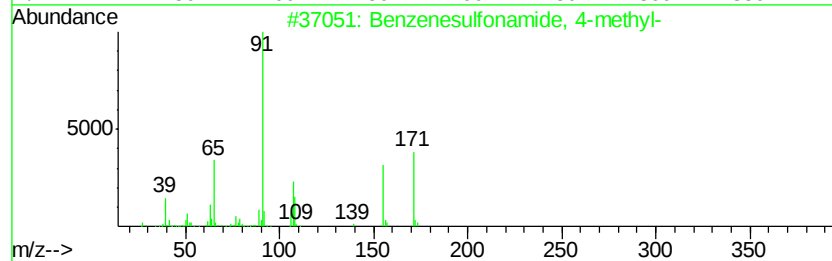
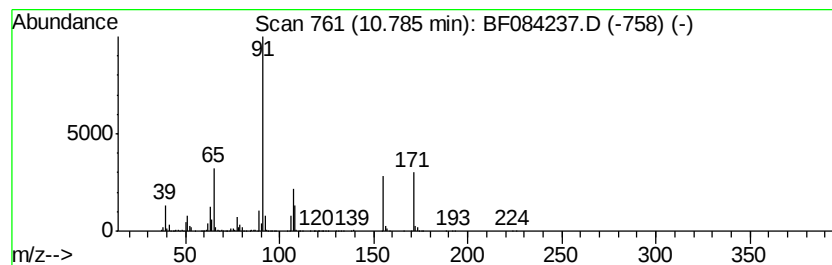
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	24.89 ng	3349890	Phenanthrene-d10	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenesulfonamide, 4-methyl-	171 C7H9NO2S	000070-55-3 98
2		Thiosulfuric acid, S-[2-[3-(4-me...	381 C12H19N3O5S3	1000255-60-3 86
3		N-p-toluenesulfonyl-L-threonine,...	363 C18H21NO5S	1000130-34-4 83
4		O-p-toluenesulfonyl-L-N-acetylser...	315 C13H17NO6S	1000126-44-8 83
5		Tolbutamide	270 C12H18N2O3S	000064-77-7 80



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Operator : UM/SJ
Sample : G4981-04
Misc :
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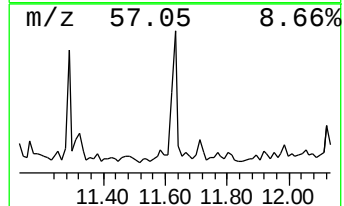
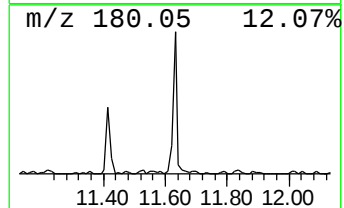
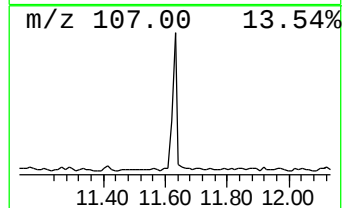
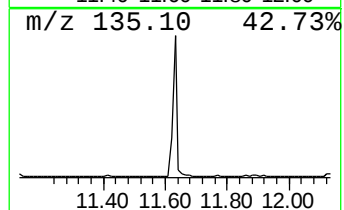
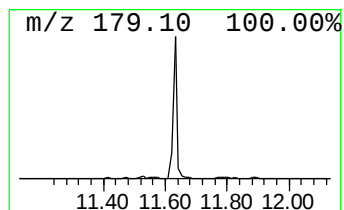
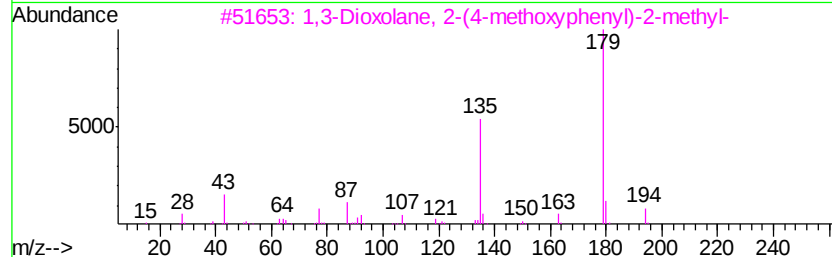
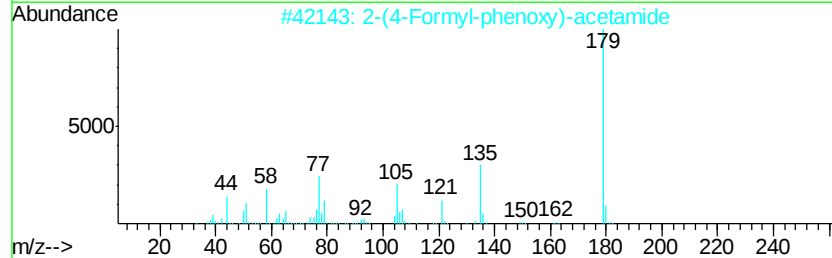
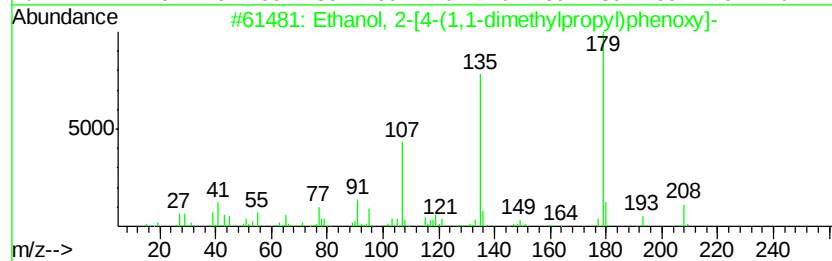
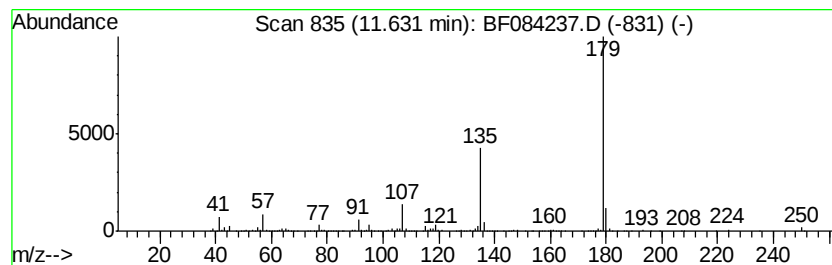
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.63	4.46 ng	601003	Phenanthrene-d10	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[4-(1,1-dimethylpropy...	208	C13H20O2	006382-07-6	78
2		2-(4-Formyl-phenoxy)-acetamide	179	C9H9NO3	135857-20-4	72
3		1,3-Dioxolane, 2-(4-methoxypheny...	194	C11H14O3	036881-00-2	64
4		Ethanol, 2-[4-(1,1-dimethylethyl...	194	C12H18O2	000713-46-2	50
5		Benzoic acid, 4-nitroso-, ethyl ...	179	C9H9NO3	007476-79-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
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ClientSampleId :
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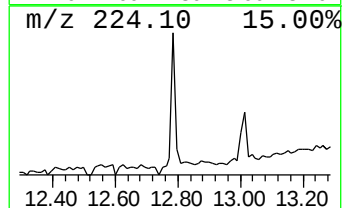
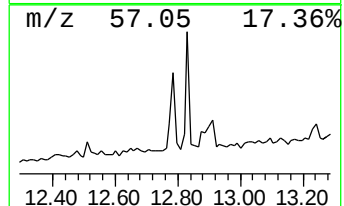
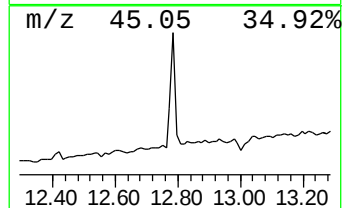
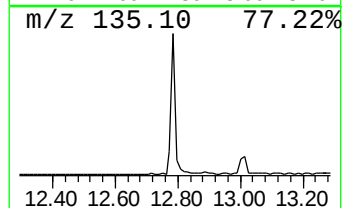
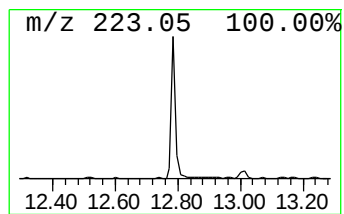
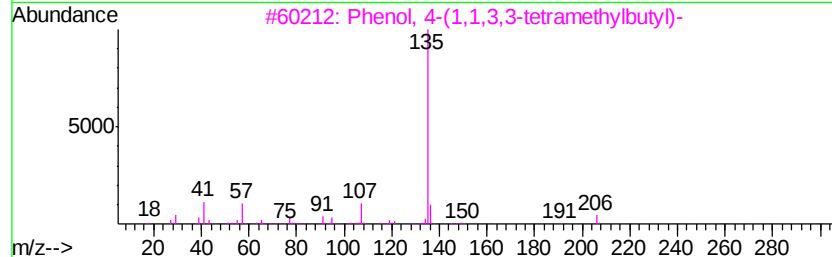
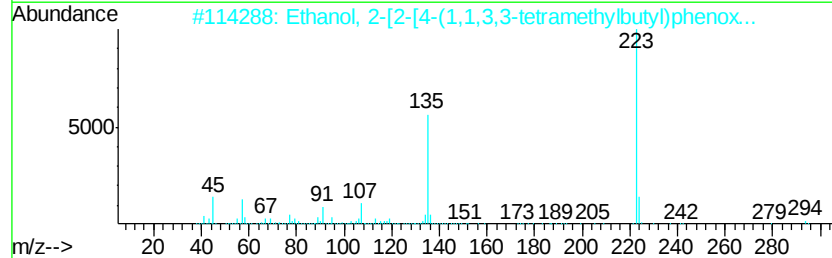
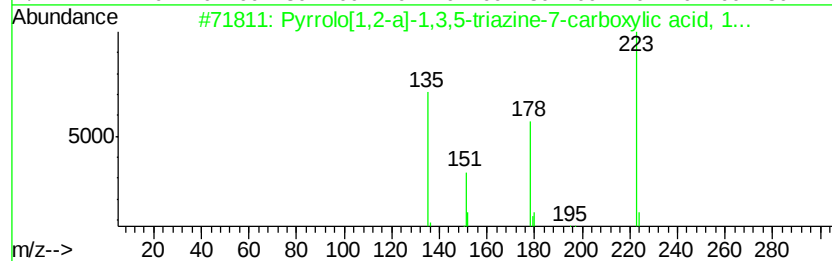
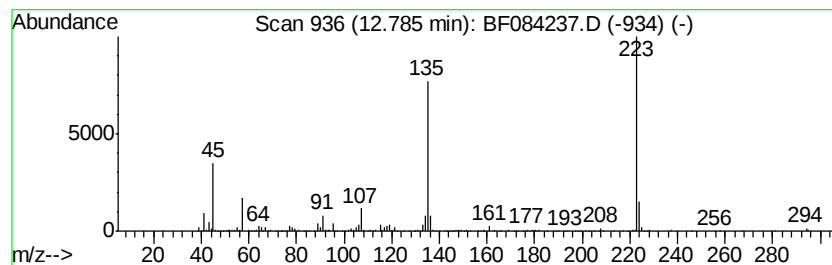
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	5.41 ng	489220	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	46
3		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	35
4		3-(p-Methoxybenzoyl)-propionic acid	208	C11H12O4	003153-44-4	35
5		1,4-Benzenediamine, N-(1-methylh...	220	C14H24N2	039563-50-3	35



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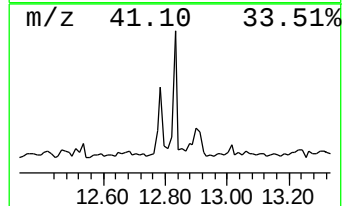
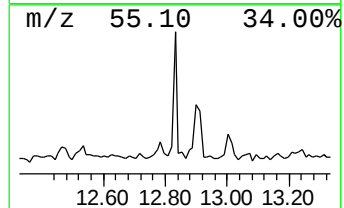
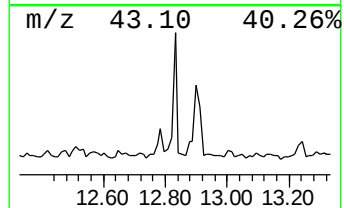
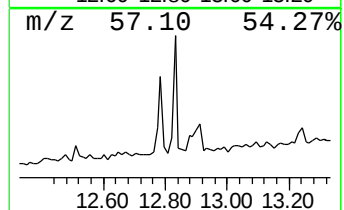
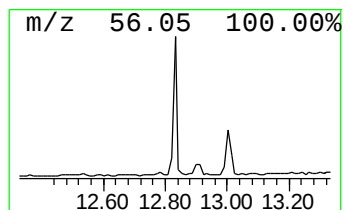
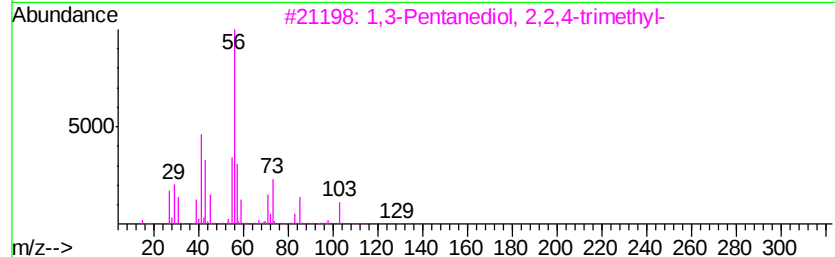
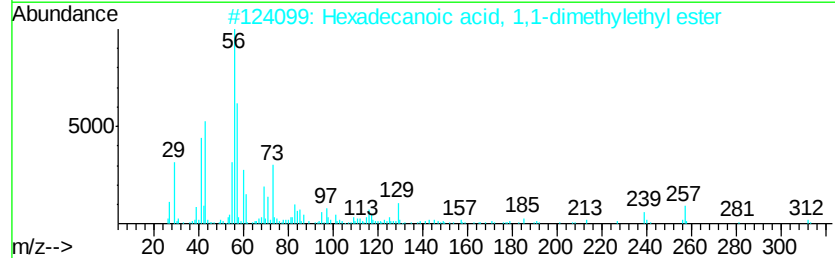
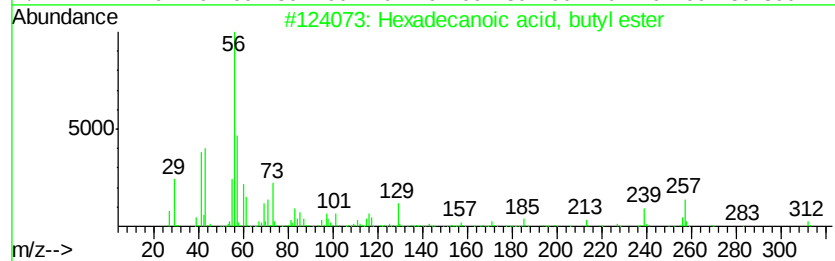
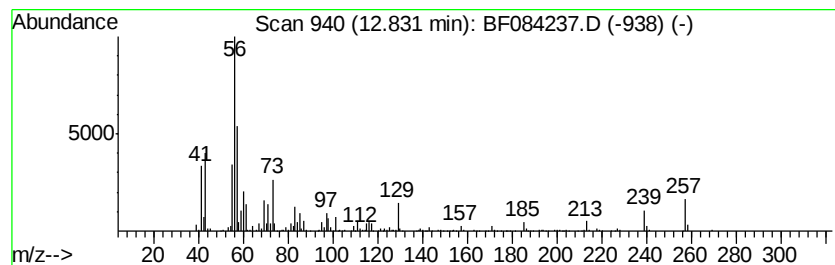
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	3.69 ng	333576	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47
4			Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084237.D
Acq On : 4 Jan 2016 14:27
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Misc :
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ClientSampleId :
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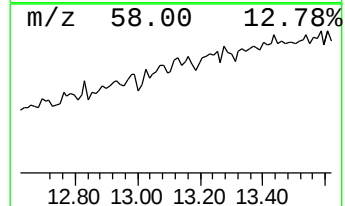
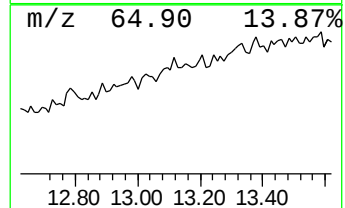
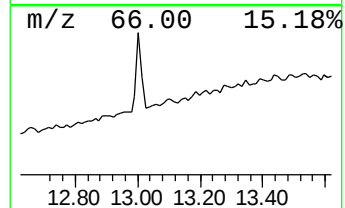
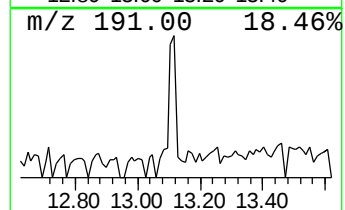
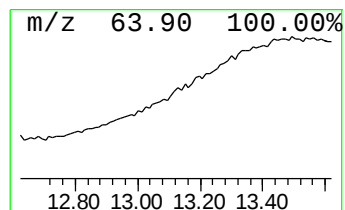
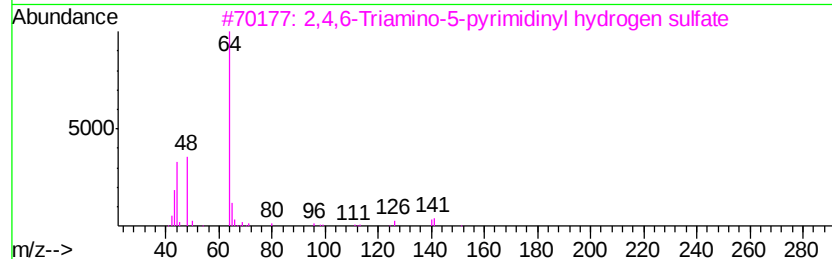
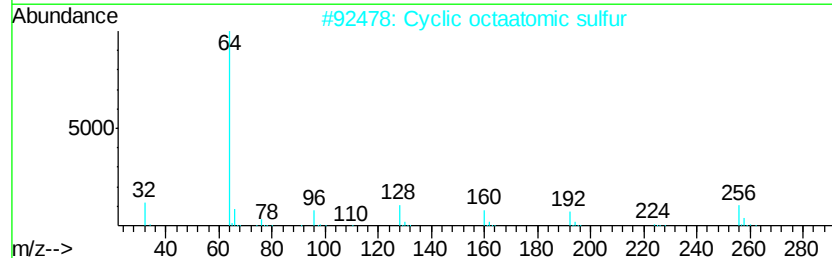
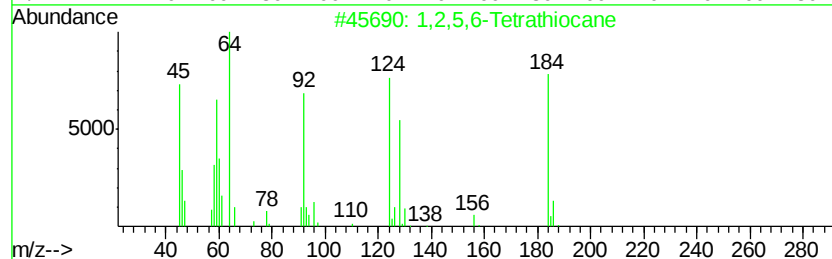
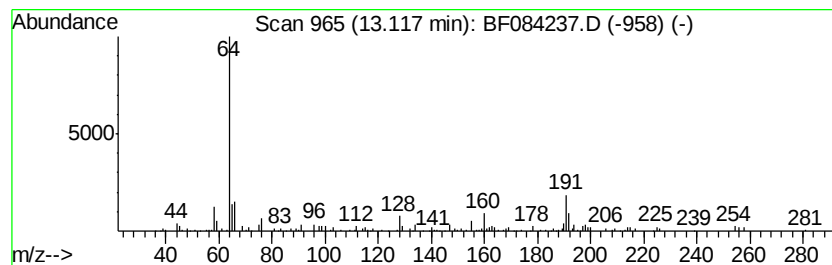
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1,2,5,6-Tetrathiocane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	2.06 ng	186134	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	78
2			Cyclic octaatomic sulfur	256	S8	010544-50-0	64
3			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	56
4			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	43
5			S-2-[2-Succinimidoethylamino]eth...	282	C8H14N2O5S2	031701-74-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
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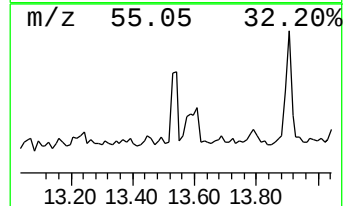
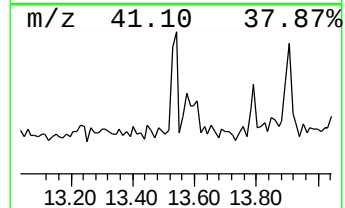
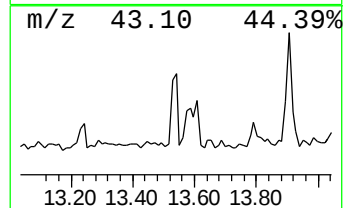
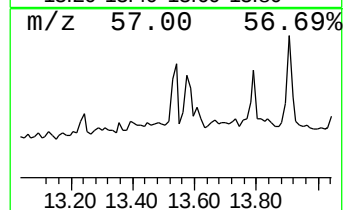
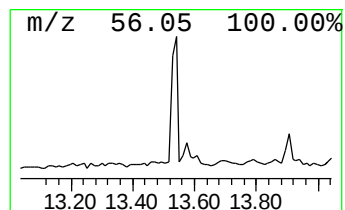
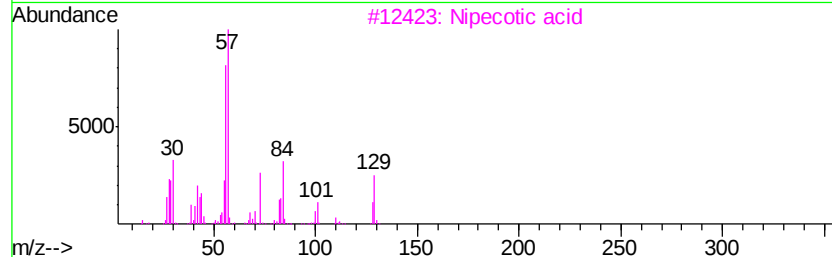
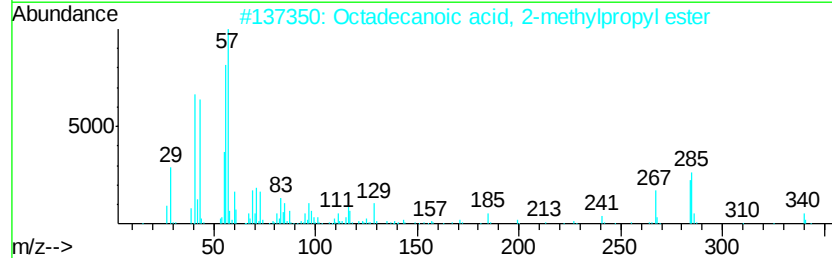
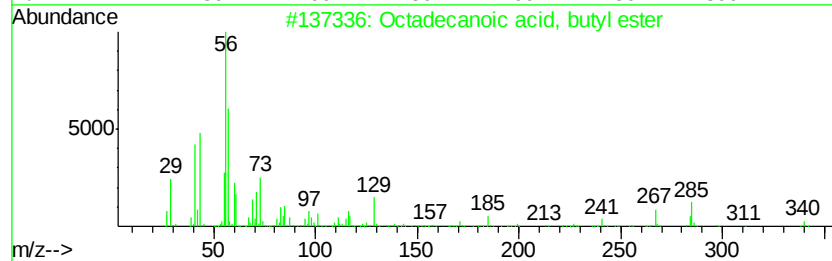
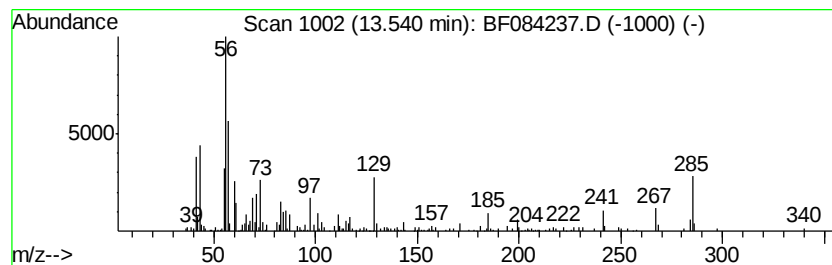
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecanoic acid, butyl ester Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	2.10 ng	190363	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	72
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	42
3		Nipecotic acid	129	C6H11NO2	000498-95-3	38
4		2-Oxazolamine, 4,5-dihydro-5-(ph...	268	C16H16N2O2	025409-59-0	35
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
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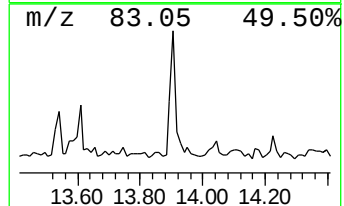
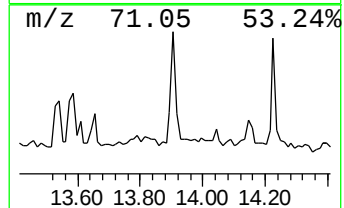
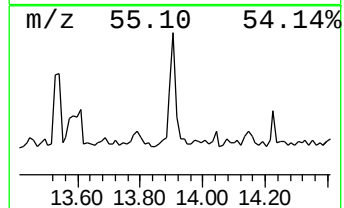
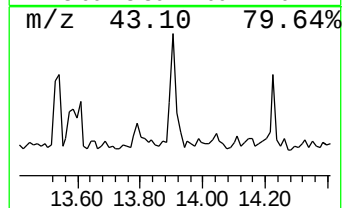
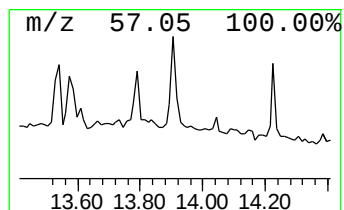
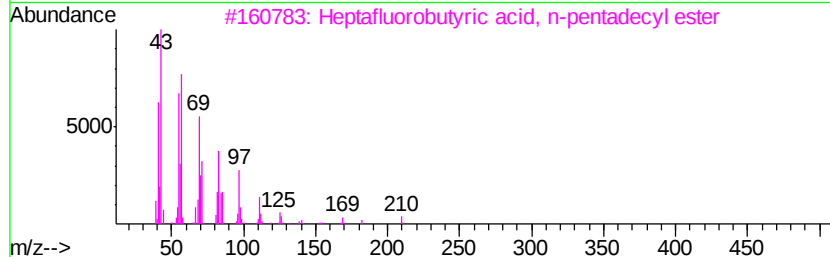
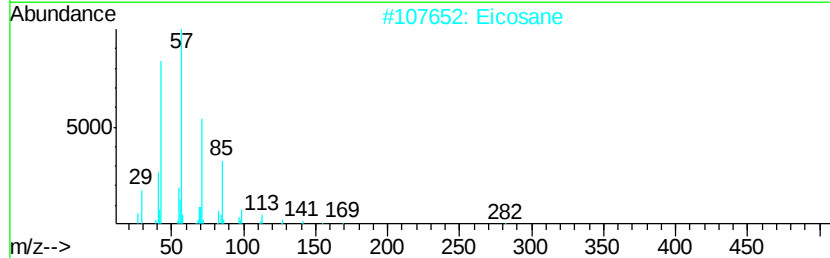
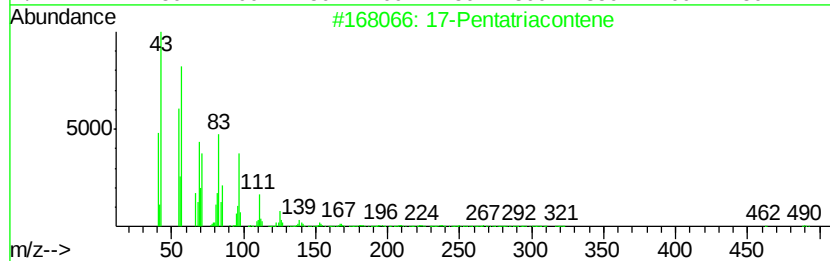
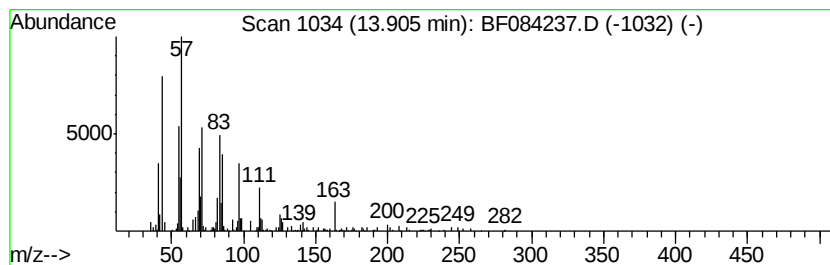
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	5.68 ng	513808	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	53
2			Eicosane	282	C20H42	000112-95-8	49
3			Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	46
4			1-Iodoundecane	282	C11H23I	004282-44-4	46
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	45



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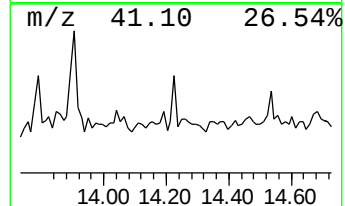
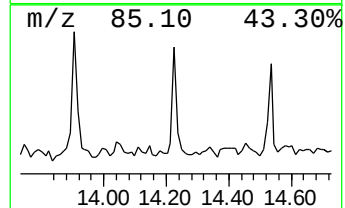
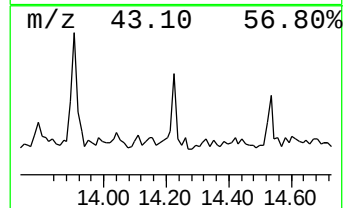
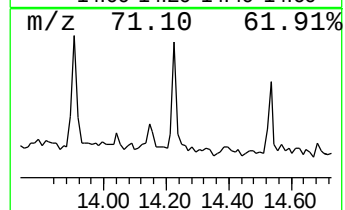
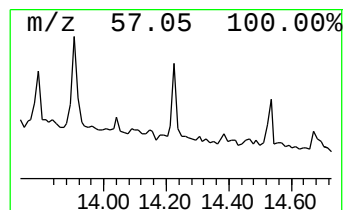
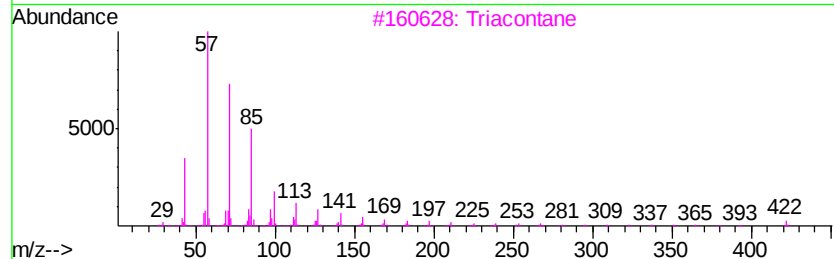
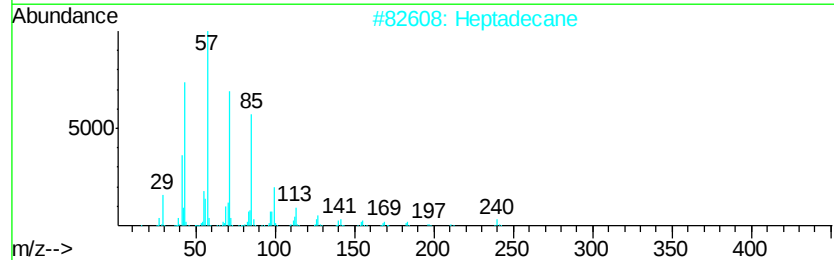
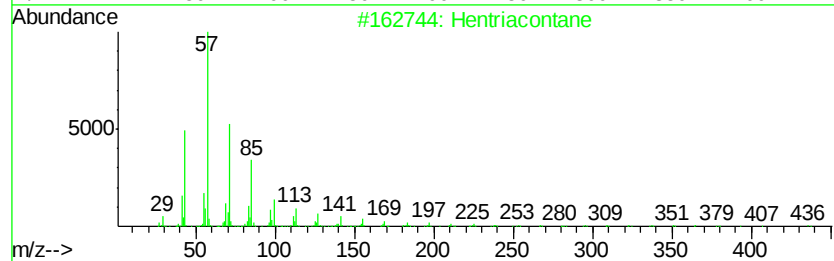
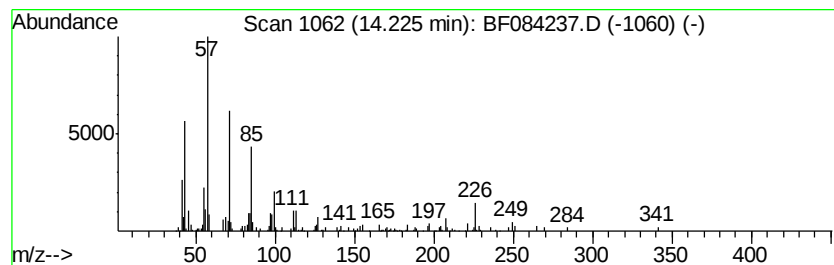
Instrument :
BNA_F
ClientSampleId :
S8-0531

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.71 ng	245227	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Hentriacontane	437 C31H64	000630-04-6 86
2		Heptadecane	240 C17H36	000629-78-7 74
3		Triacontane	422 C30H62	000638-68-6 72
4		Hexadecane	226 C16H34	000544-76-3 72
5		Octadecane	254 C18H38	000593-45-3 64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084237.D
Acq On : 4 Jan 2016 14:27
Operator : UM/SJ
Sample : G4981-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0531

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	10.3	ng	1083450	1	6.89	2112120	20.0
unknown6.66	6.66	63.7	ng	6728520	1	6.89	2112120	20.0
Hexadecane	10.36	2.3	ng	330513	3	9.93	2871600	20.0
Benzenesulfonamid...	10.59	19.9	ng	2854280	3	9.93	2871600	20.0
Benzenesulfonamid...	10.79	24.9	ng	3349890	4	11.41	2692220	20.0
Ethanol, 2-[4-(1,...	11.63	4.5	ng	601003	4	11.41	2692220	20.0
Pyrrolo[1,2-a]-1,...	12.79	5.4	ng	489220	5	14.05	1809720	20.0
Hexadecanoic acid...	12.83	3.7	ng	333576	5	14.05	1809720	20.0
1,2,5,6-Tetrathio...	13.12	2.1	ng	186134	5	14.05	1809720	20.0
Octadecanoic acid...	13.54	2.1	ng	190363	5	14.05	1809720	20.0
17-Pentatriacontene	13.91	5.7	ng	513808	5	14.05	1809720	20.0
Hentriacontane	14.23	2.7	ng	245227	5	14.05	1809720	20.0