

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
 Data File : BF076950.D
 Acq On : 20 Jan 2015 5:10
 Operator : IZ / TP
 Sample : G1080-06
 Misc : W
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-PMW-2-15

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-BF011415.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	1.464	31	33	44	rVB	25559	59591	4.17%	0.583%
2	4.104	261	264	273	rBV	43351	96251	6.73%	0.941%
3	5.041	344	346	363	rVB	218811	467562	32.70%	4.573%
4	7.384	548	551	556	rBV	124052	260536	18.22%	2.548%
5	7.476	556	559	567	rVB	525814	959451	67.11%	9.384%
6	7.967	599	602	607	rVB	125802	215896	15.10%	2.111%
7	8.299	627	631	634	rBV	532399	883800	61.82%	8.644%
8	9.270	712	716	719	rBV	482146	715264	50.03%	6.995%
9	9.316	719	720	725	rVB	14615	17949	1.26%	0.176%
10	10.882	853	857	861	rBV	196850	295728	20.68%	2.892%
11	13.534	1085	1089	1092	rBV	954419	1429729	100.00%	13.983%
12	15.008	1215	1218	1222	rBV	215453	324347	22.69%	3.172%
13	16.677	1361	1364	1367	rBV	620031	861950	60.29%	8.430%
14	17.774	1457	1460	1463	rBV	288867	333837	23.35%	3.265%
15	18.757	1544	1546	1549	rBV	43918	62291	4.36%	0.609%
16	18.906	1557	1559	1564	rBV3	9859	25934	1.81%	0.254%
17	19.466	1606	1608	1611	rBV	90441	109985	7.69%	1.076%
18	19.786	1633	1636	1638	rBV2	13011	18393	1.29%	0.180%
19	19.900	1643	1646	1649	rVB	144628	149472	10.45%	1.462%
20	20.003	1653	1655	1658	rVB	1249147	1390827	97.28%	13.603%
21	20.414	1689	1691	1695	rVB3	8117	16961	1.19%	0.166%
22	20.792	1721	1724	1726	rVB	116144	129971	9.09%	1.271%
23	20.849	1726	1729	1731	rBV	22164	31187	2.18%	0.305%
24	20.929	1734	1736	1740	rVV	14537	17636	1.23%	0.172%
25	21.146	1753	1755	1757	rBV	58775	97110	6.79%	0.950%
26	21.180	1757	1758	1761	rVB	123789	156169	10.92%	1.527%
27	21.272	1761	1766	1769	rBV	342373	428362	29.96%	4.189%
28	21.397	1774	1777	1780	rBV	18950	30833	2.16%	0.302%
29	21.660	1797	1800	1803	rVB	33800	46660	3.26%	0.456%
30	22.037	1831	1833	1837	rVB	26940	33834	2.37%	0.331%
31	22.415	1863	1866	1868	rVB	21567	32567	2.28%	0.319%
32	22.780	1895	1898	1904	rVB3	16046	29269	2.05%	0.286%
33	22.917	1907	1910	1913	rBV	245183	311673	21.80%	3.048%
34	23.135	1926	1929	1932	rVB	22209	30967	2.17%	0.303%

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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-BF011415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.489	1957	1960	1963	rBV4	16572	35683	2.50%	0.349%
36	23.786	1984	1986	1989	rBV3	10940	20977	1.47%	0.205%
37	23.855	1989	1992	1999	rVB6	9986	29155	2.04%	0.285%
38	24.483	2044	2047	2051	rBV3	24966	50045	3.50%	0.489%
39	24.563	2051	2054	2058	rVB5	6639	16927	1.18%	0.166%

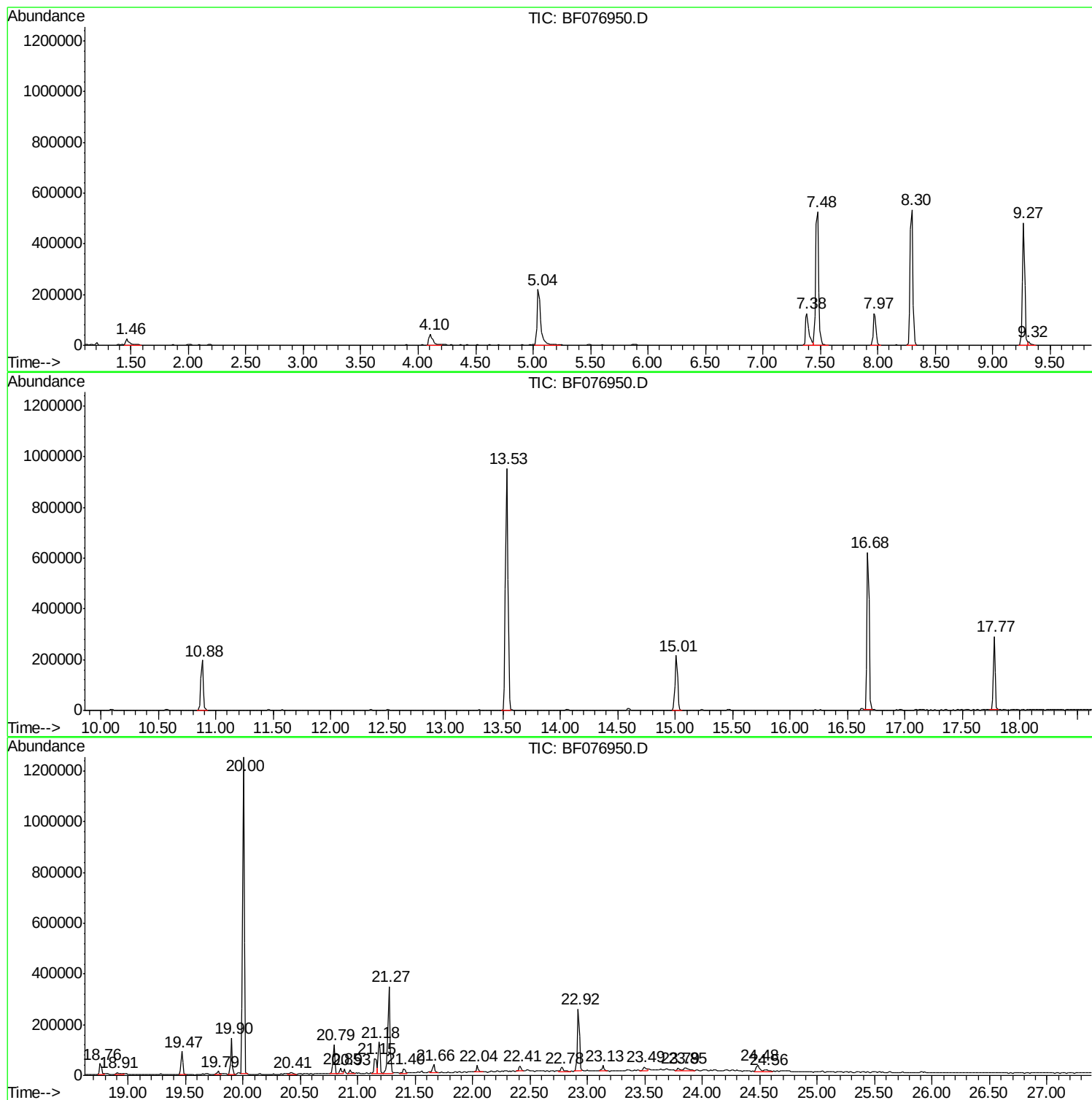
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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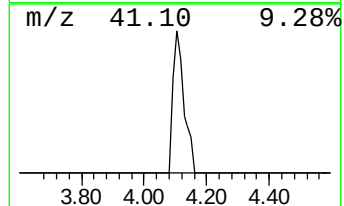
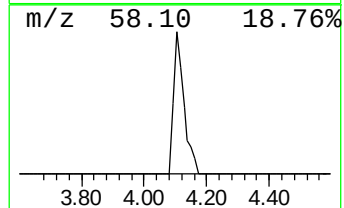
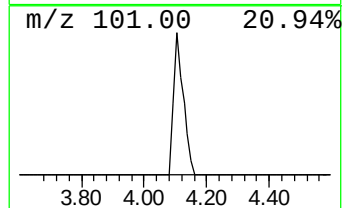
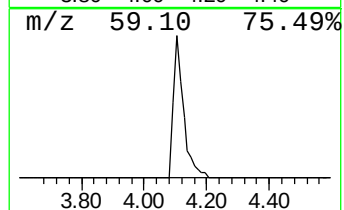
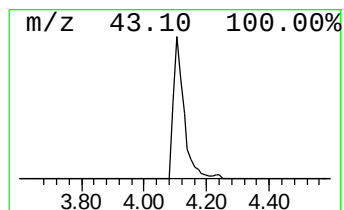
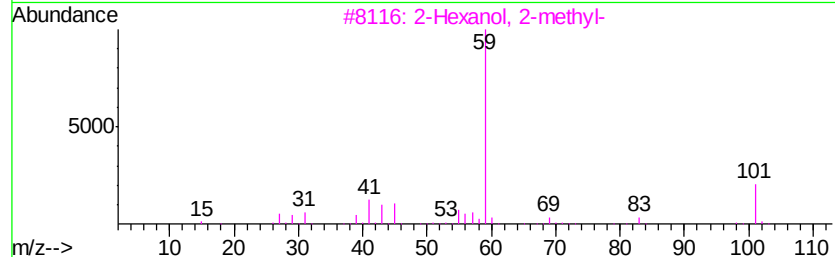
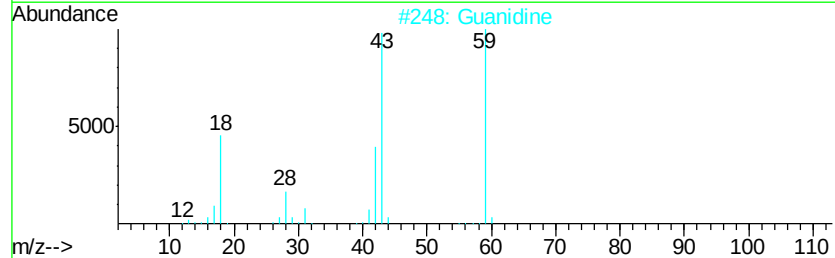
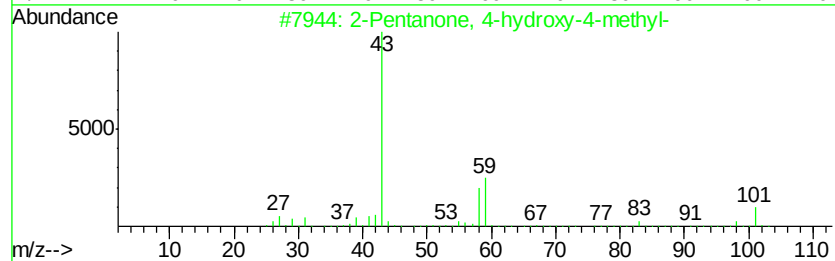
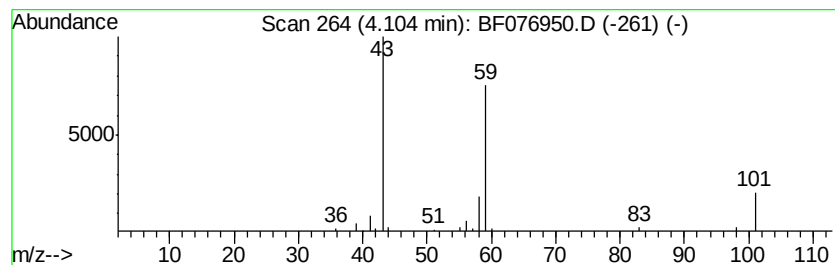
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	8.92 ng	96251	1,4-Dichlorobenzene-d4	7.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	53
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	33
5			Acetone	58	C3H6O	000067-64-1	9



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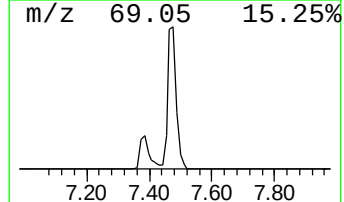
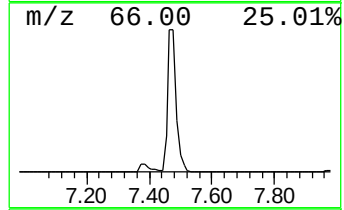
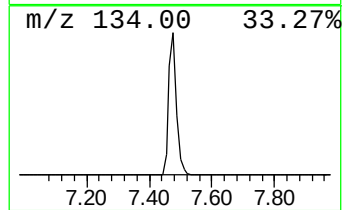
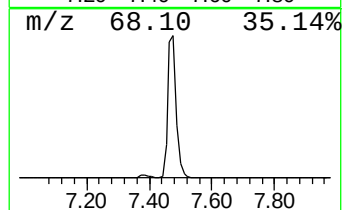
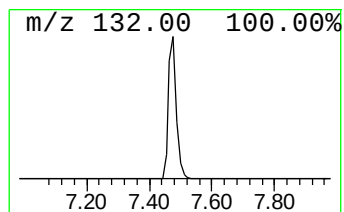
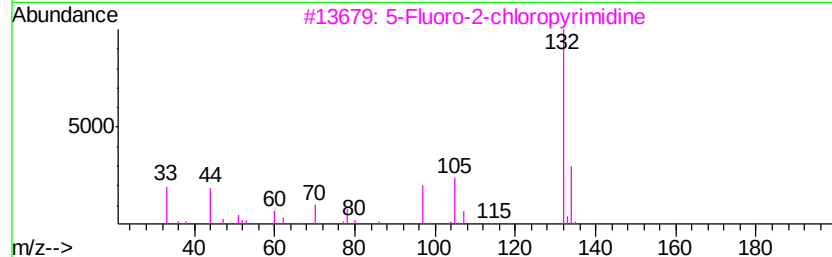
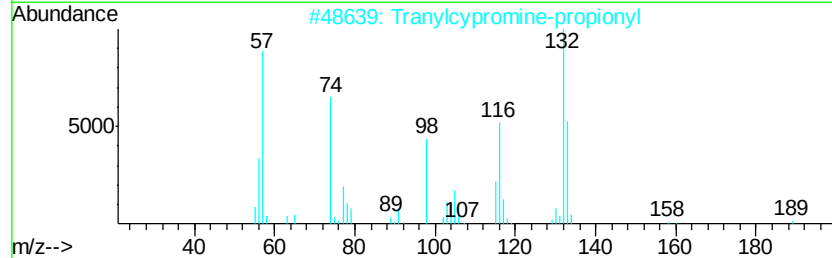
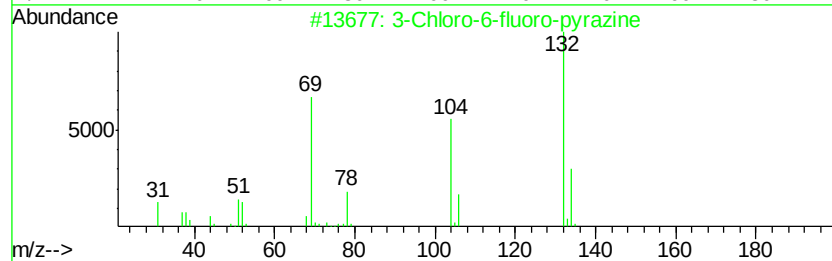
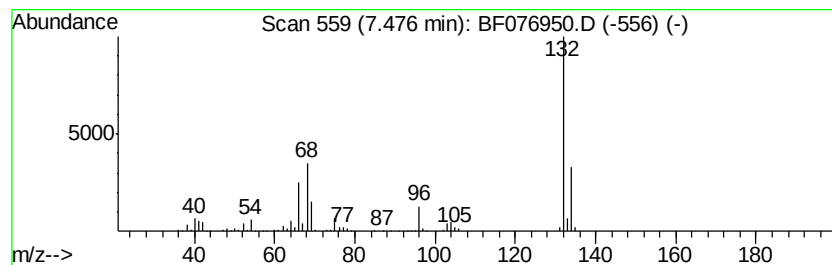
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	88.88 ng	959451	1,4-Dichlorobenzene-d4	7.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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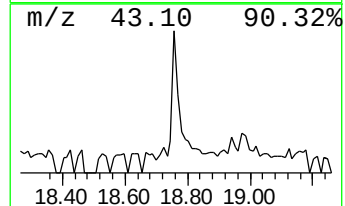
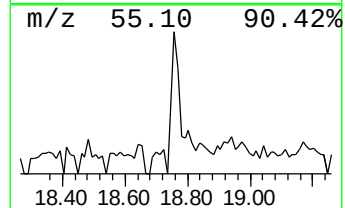
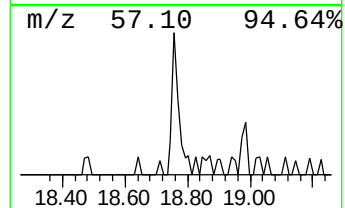
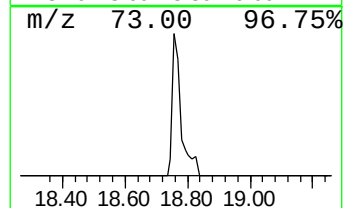
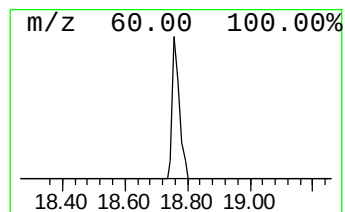
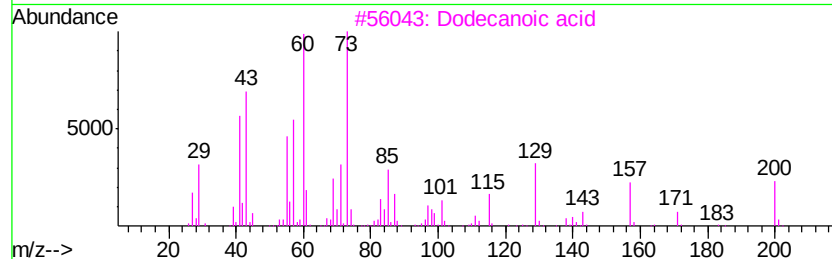
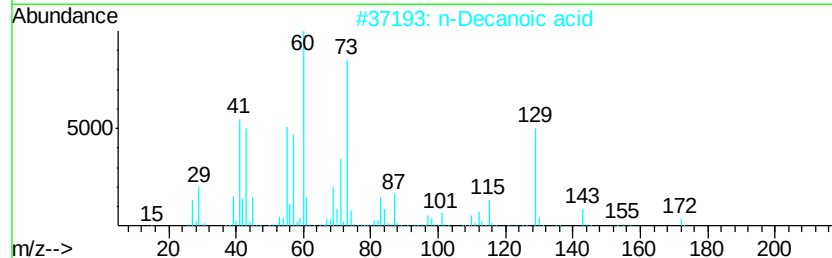
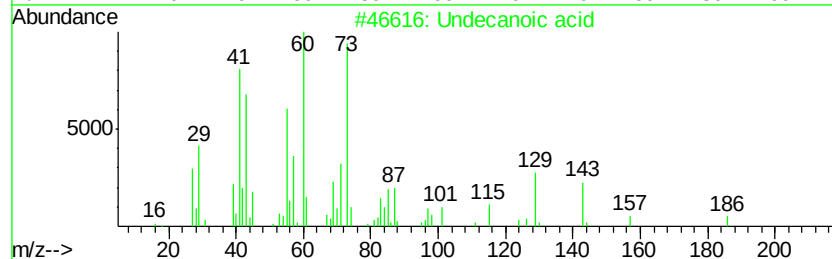
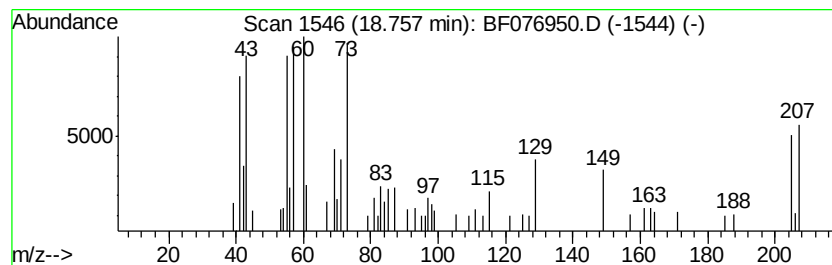
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown18.76 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	3.73 ng	62291	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	43
2		n-Decanoic acid	172	C10H20O2	000334-48-5	38
3		Dodecanoic acid	200	C12H24O2	000143-07-7	32
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	27
5		.alpha.-D-Galactopyranoside, met...	306	C15H30O6	1000157-05-0	25



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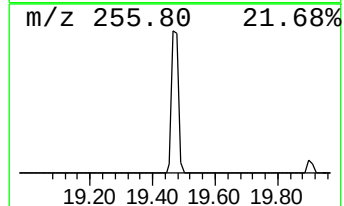
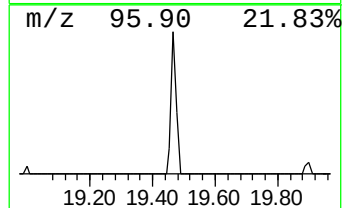
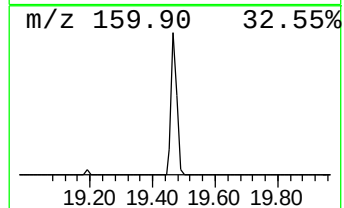
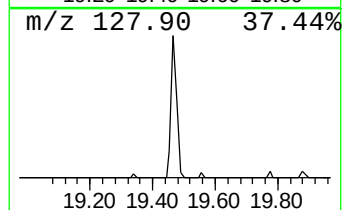
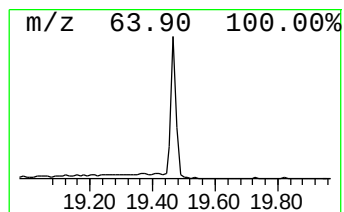
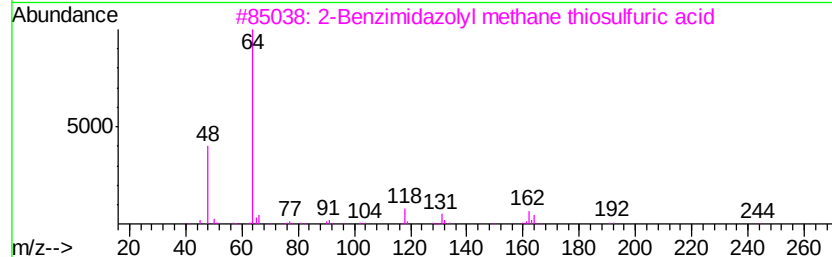
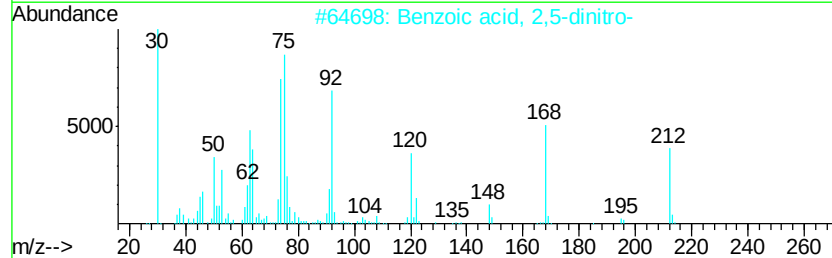
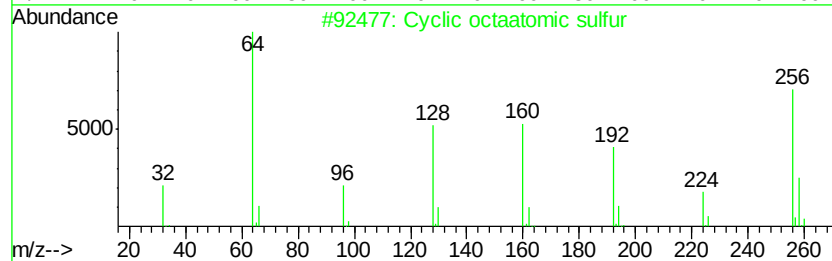
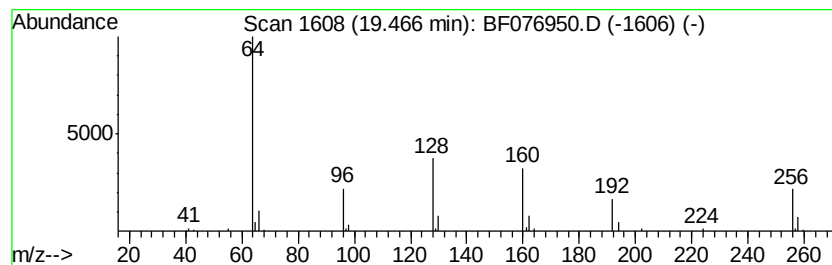
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclic octaatomic sulfur Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	6.59 ng	109985	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2		Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	53
3		2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1000256-39-2	9
4		2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	9
5		1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9



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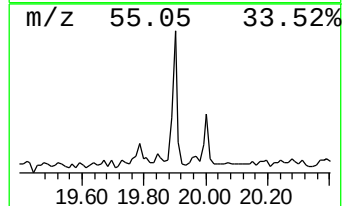
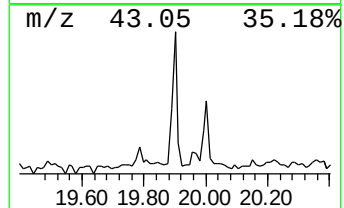
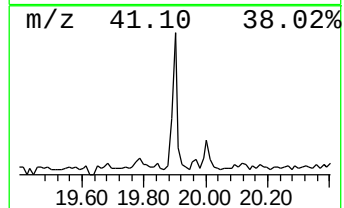
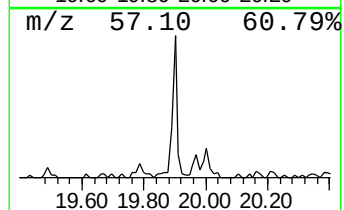
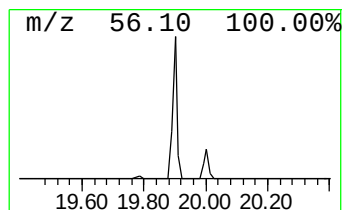
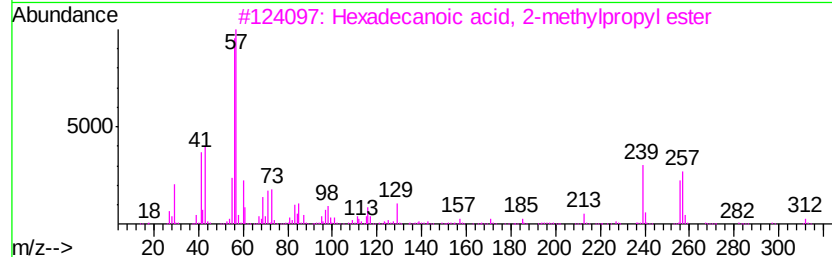
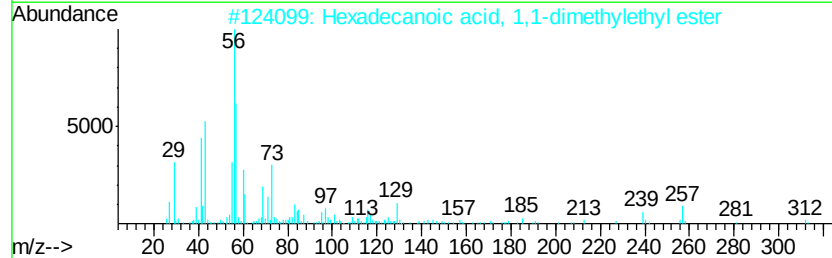
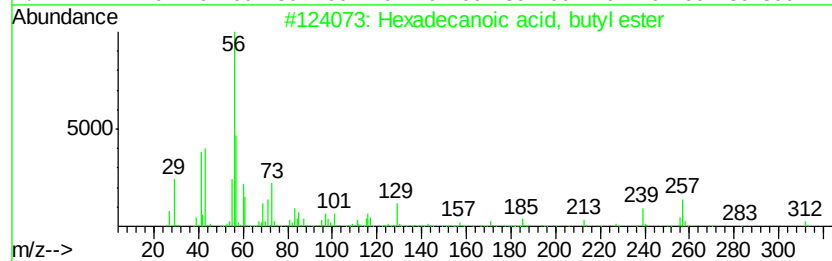
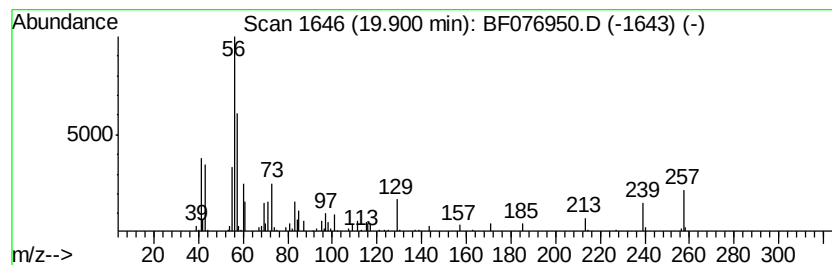
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	6.98 ng	149472	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	59
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
Operator : IZ / TP
Sample : G1080-06
Misc : W
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TE-PMW-2-15

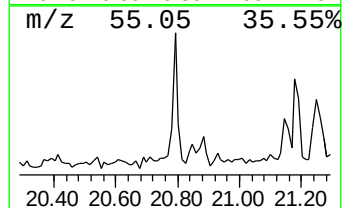
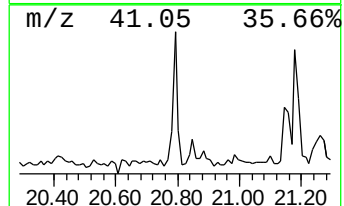
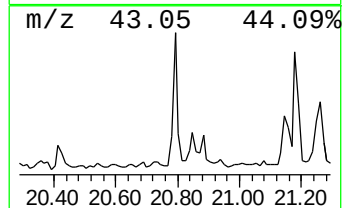
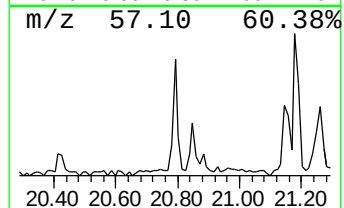
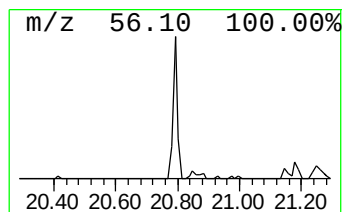
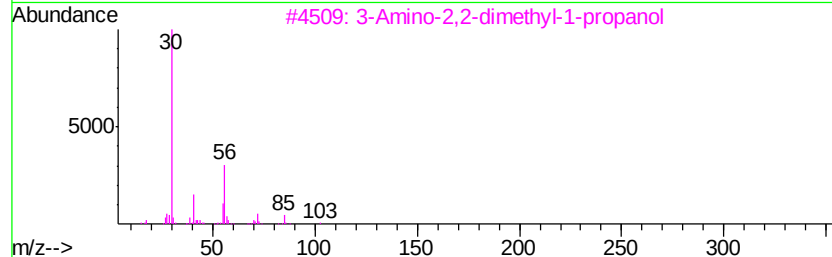
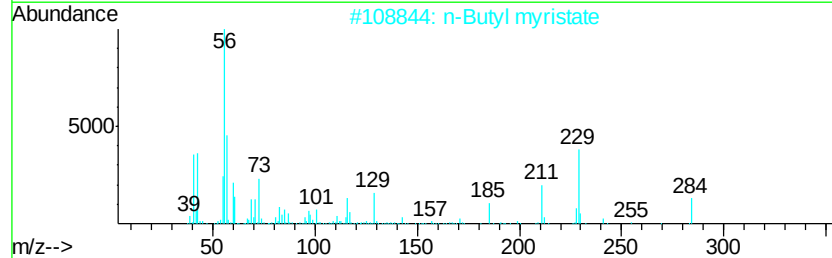
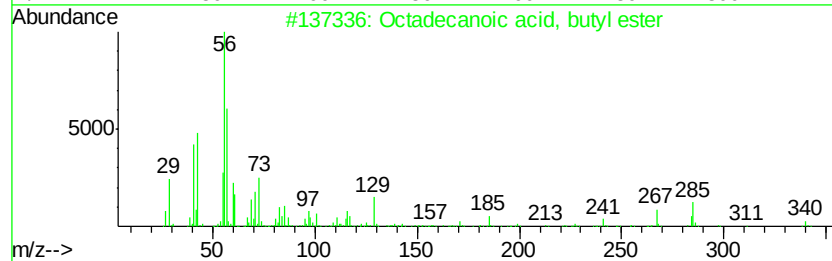
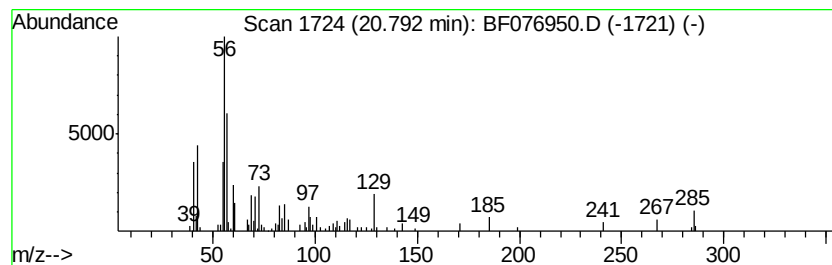
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	6.07 ng	129971	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	38
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
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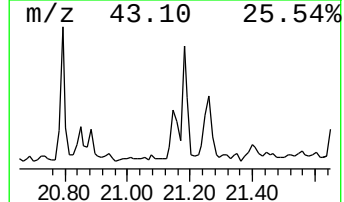
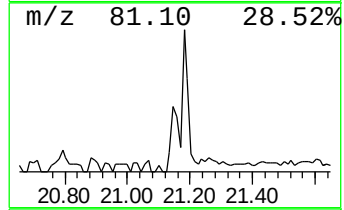
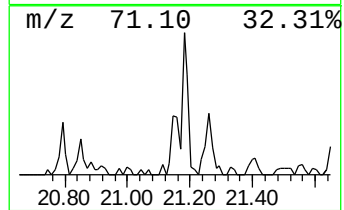
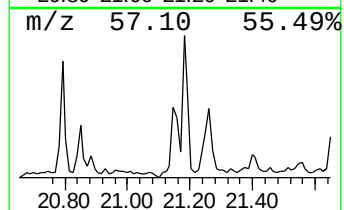
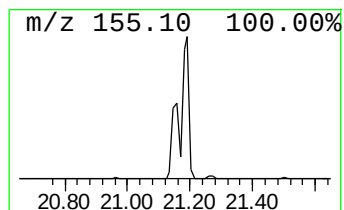
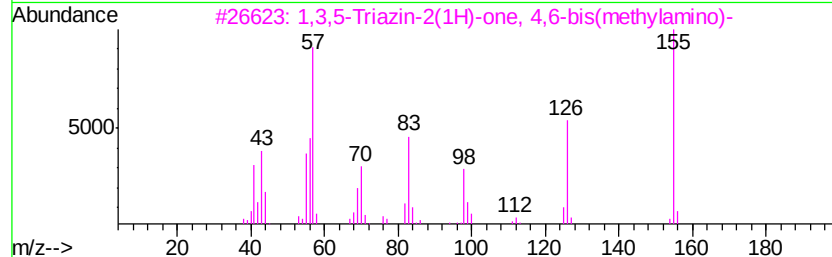
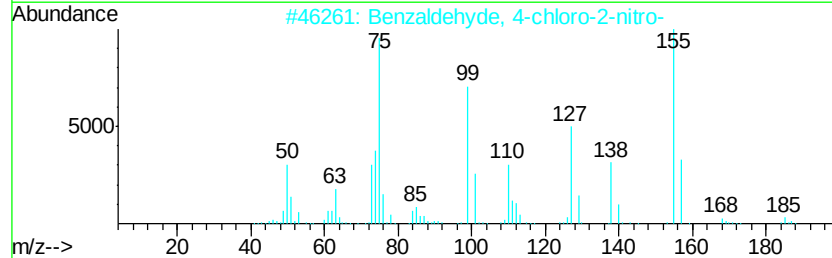
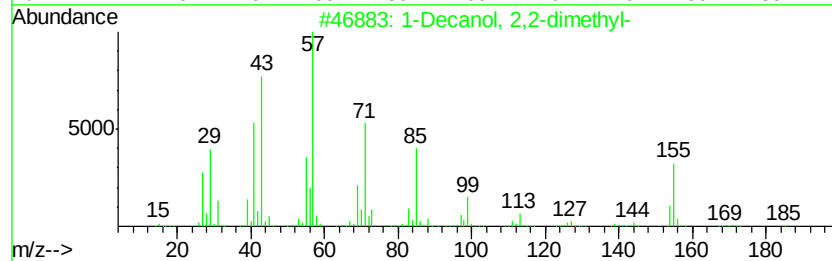
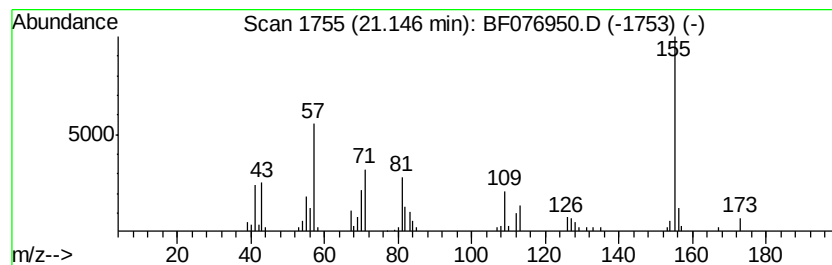
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.15 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	4.53 ng	97110	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	40
2		Benzaldehyde, 4-chloro-2-nitro-	185	C7H4ClNO3	005551-11-1	38
3		1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	37
4		4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	32
5		2,4-Diethyl-5-methylthiazole	155	C8H13NS	052414-89-8	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
Operator : IZ / TP
Sample : G1080-06
Misc : W
ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
TE-PMW-2-15

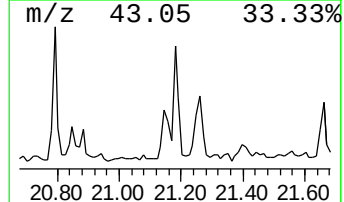
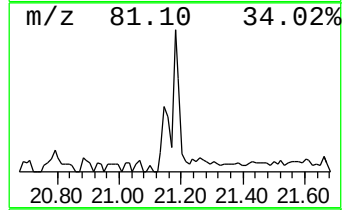
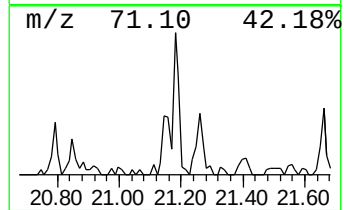
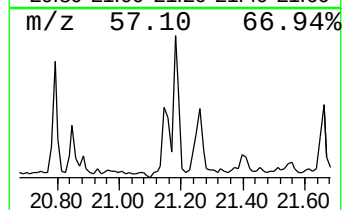
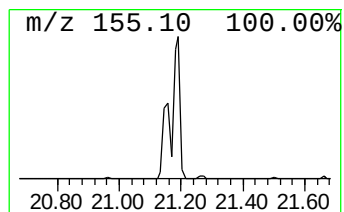
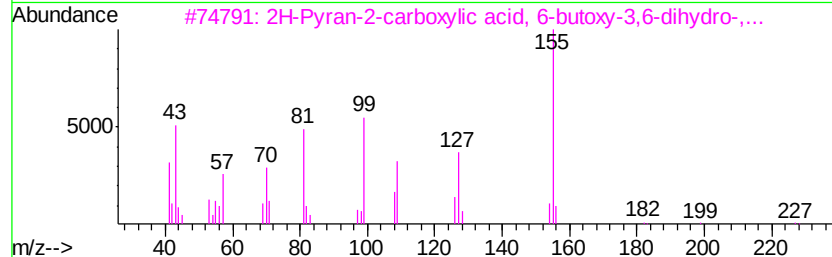
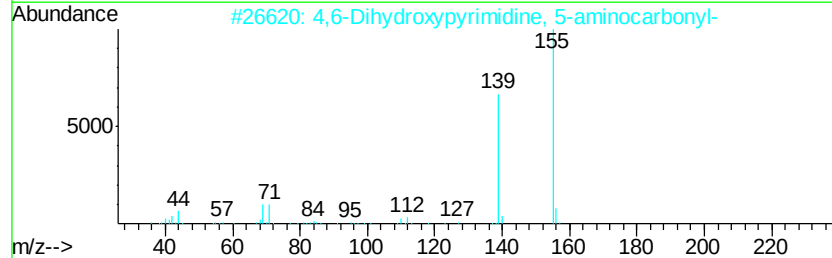
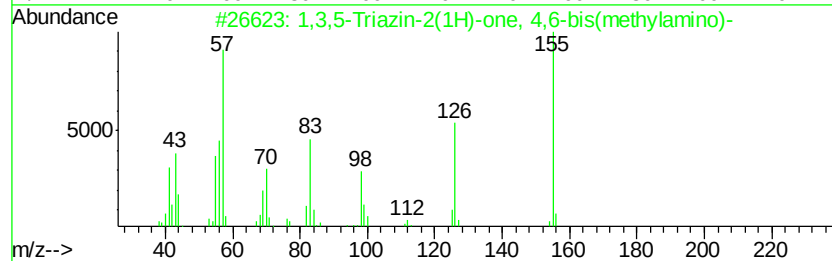
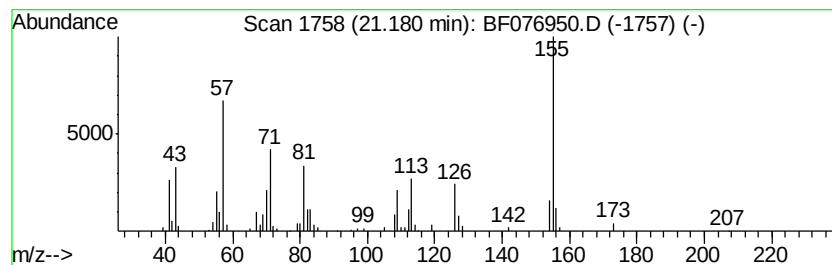
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown21.18 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.18	7.29 ng	156169	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	38
2		4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	27
3		2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	25
4		[1,1'-Bicyclohexyl]-1,1'-diol, 3...	310	C20H38O2	068525-22-4	16
5		2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
Operator : IZ / TP
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Misc : W
ALS Vial : 27 Sample Multiplier: 1

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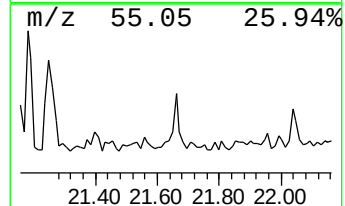
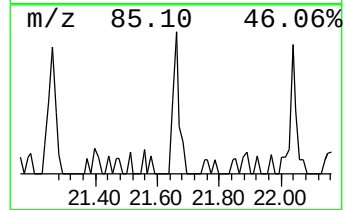
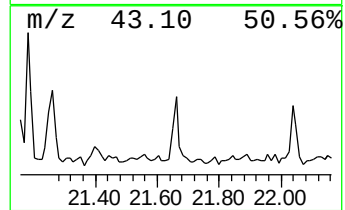
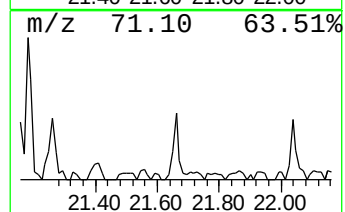
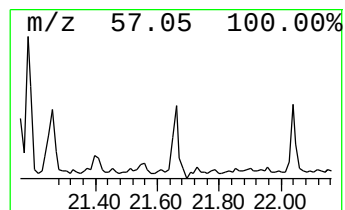
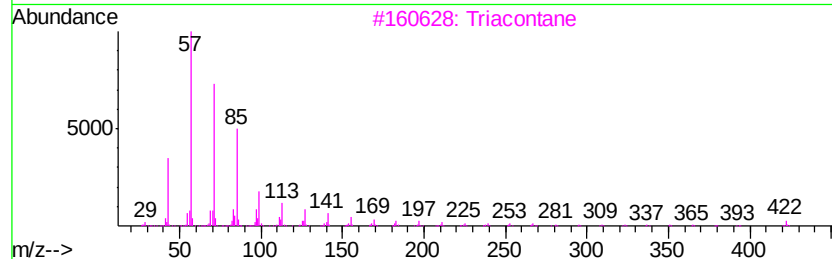
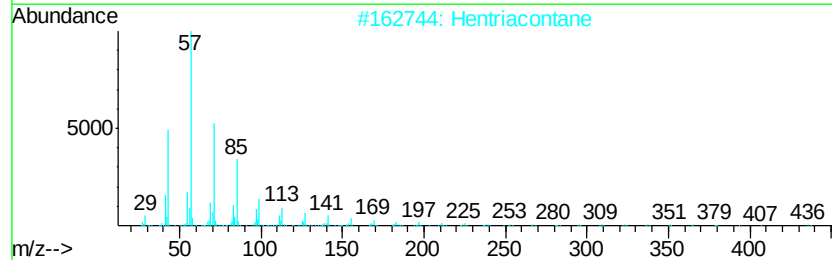
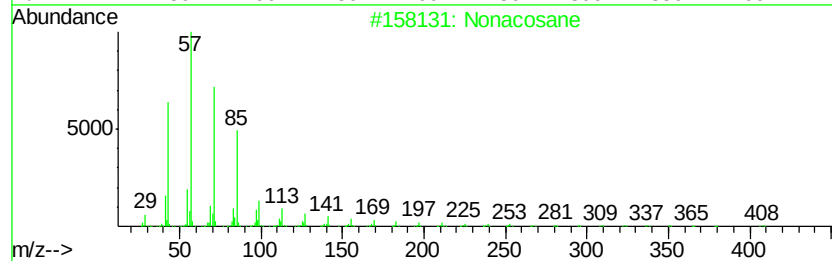
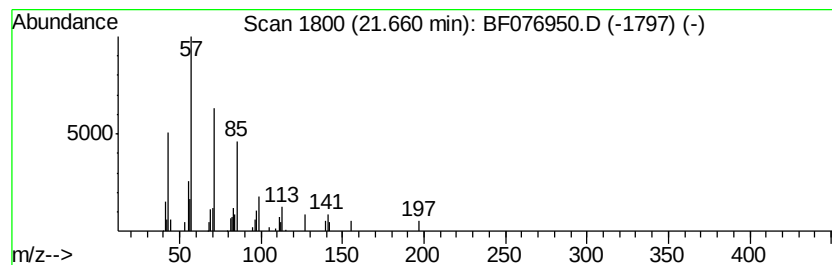
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.66	2.18 ng	46660	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonacosane	408	C29H60	000630-03-5	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Triacontane	422	C30H62	000638-68-6	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
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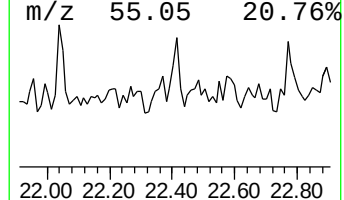
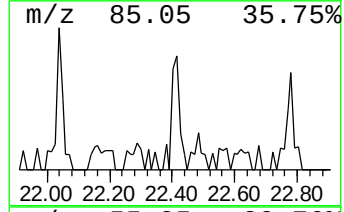
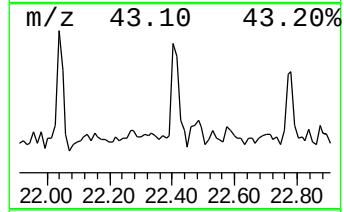
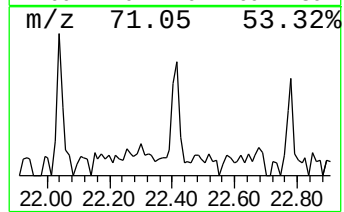
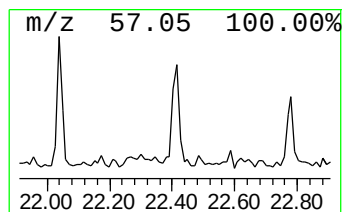
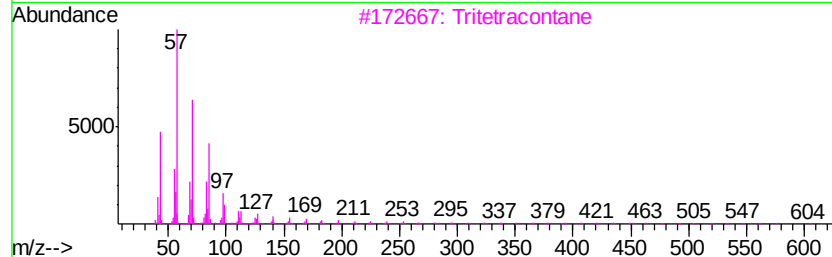
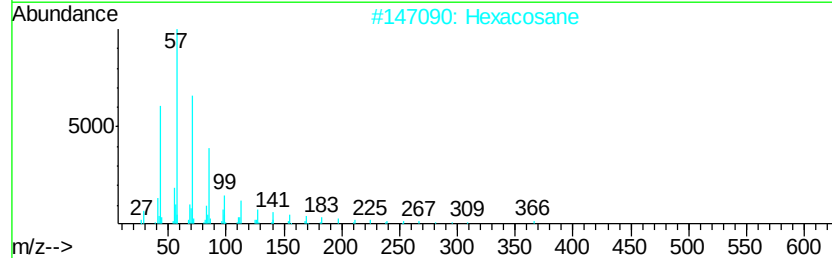
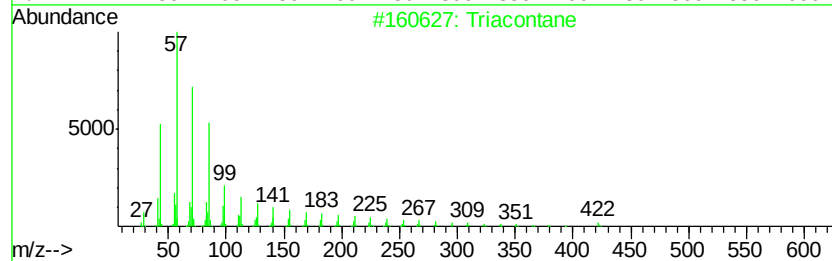
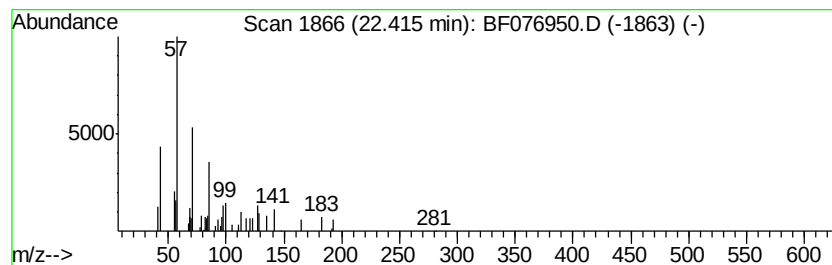
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Triacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.09 ng	32567	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	78
2		Hexacosane	366	C26H54	000630-01-3	64
3		Tritetracontane	605	C43H88	007098-21-7	64
4		Octadecane	254	C18H38	000593-45-3	59
5		Nonadecane	268	C19H40	000629-92-5	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
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Sample : G1080-06
Misc : W
ALS Vial : 27 Sample Multiplier: 1

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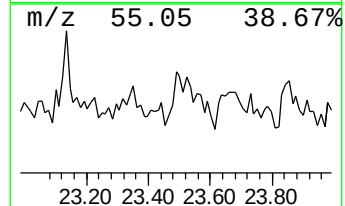
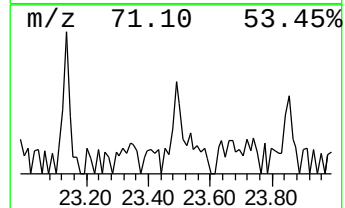
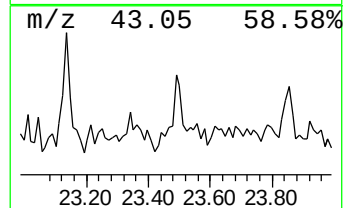
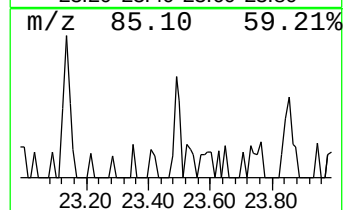
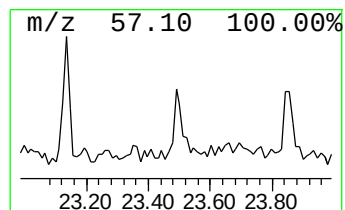
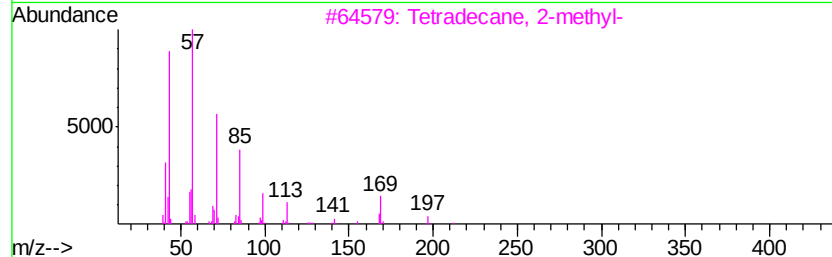
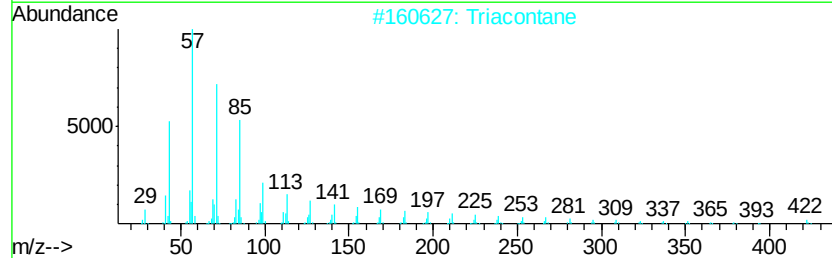
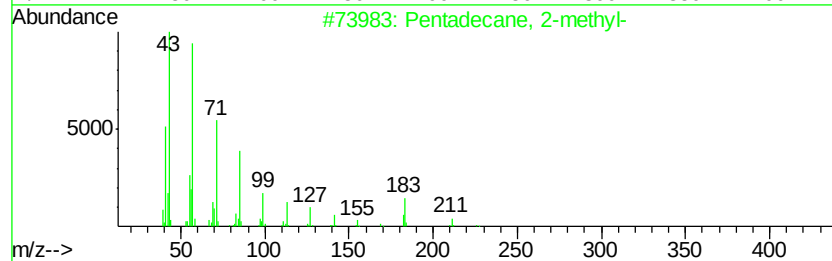
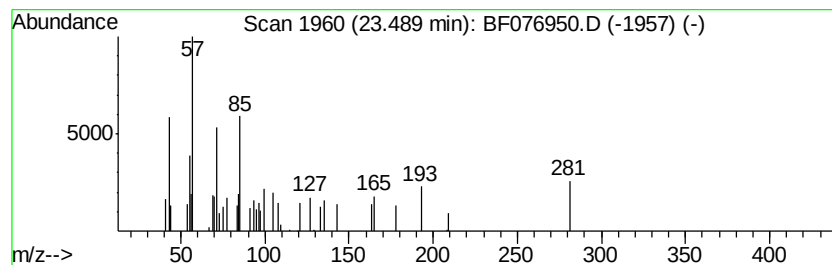
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown23.49 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.49	2.29 ng	35683	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	38
2		Triacotane	422	C30H62	000638-68-6	38
3		Tetradecane, 2-methyl-	212	C15H32	001560-95-8	38
4		Octadecane	254	C18H38	000593-45-3	38
5		Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
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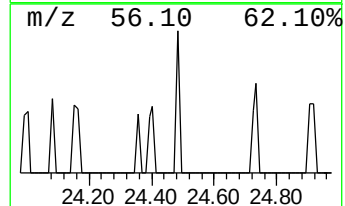
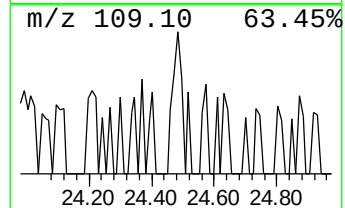
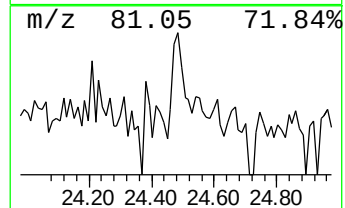
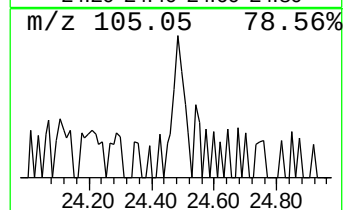
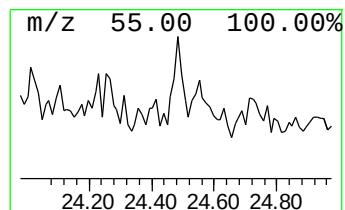
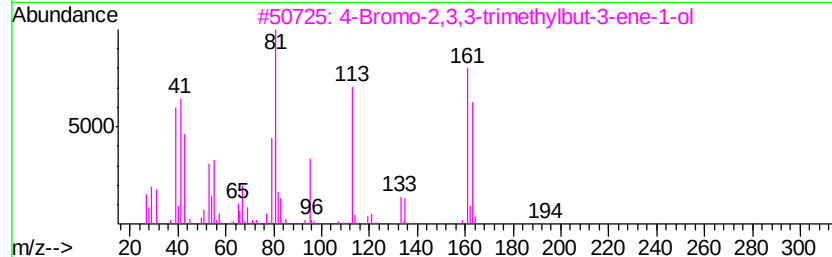
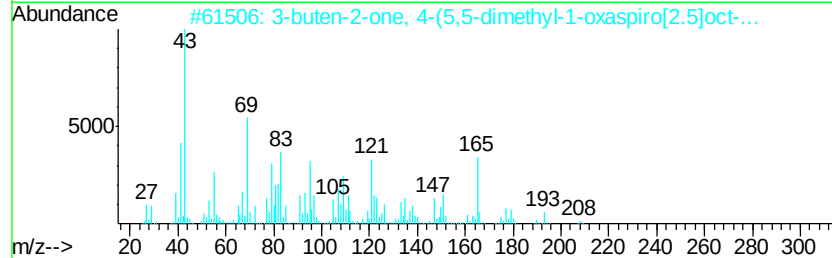
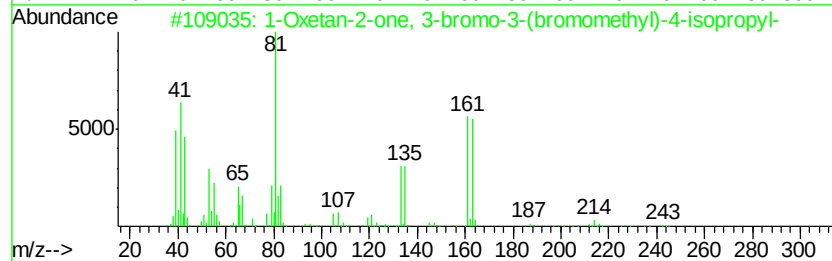
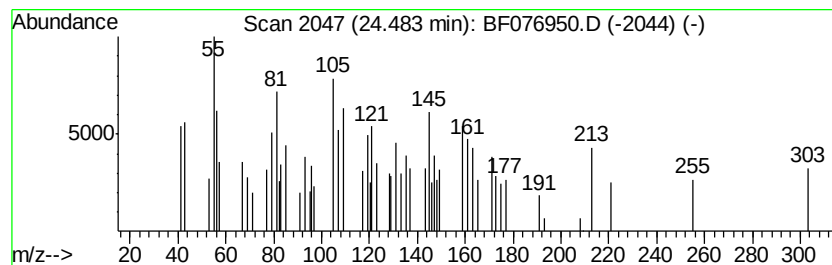
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown24.48 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.48	3.21 ng	50045	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Oxetan-2-one, 3-bromo-3-(bromo...	284	C7H10Br2O2	1000142-30-2	14
2		3-buten-2-one, 4-(5,5-dimethyl-1...	208	C13H20O2	1000196-66-5	11
3		4-Bromo-2,3,3-trimethylbut-3-ene...	192	C7H13BrO	1000222-07-2	10
4		Carbamic acid, (4-chlorophenyl)-...	213	C10H12ClNO2	002239-92-1	9
5		1,3,5-Trisilacyclohexane, 1-methyl-	146	C4H14Si3	018148-11-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076950.D
Acq On : 20 Jan 2015 5:10
Operator : IZ / TP
Sample : G1080-06
Misc : W
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-PMW-2-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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...	4.10	8.9	ng	96251	1	7.97	215896	20.0
unknown7.48	7.48	88.9	ng	959451	1	7.97	215896	20.0
unknown18.76	18.76	3.7	ng	62291	4	17.77	333837	20.0
Cyclic octaatomic...	19.47	6.6	ng	109985	4	17.77	333837	20.0
Hexadecanoic acid...	19.90	7.0	ng	149472	5	21.27	428362	20.0
Octadecanoic acid...	20.79	6.1	ng	129971	5	21.27	428362	20.0
unknown21.15	21.15	4.5	ng	97110	5	21.27	428362	20.0
unknown21.18	21.18	7.3	ng	156169	5	21.27	428362	20.0
Nonacosane	21.66	2.2	ng	46660	5	21.27	428362	20.0
triacontane	22.41	2.1	ng	32567	6	22.92	311673	20.0
unknown23.49	23.49	2.3	ng	35683	6	22.92	311673	20.0
unknown24.48	24.48	3.2	ng	50045	6	22.92	311673	20.0