

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
 Data File : BF083239.D
 Acq On : 24 Nov 2015 16:19
 Operator : UM/IZ
 Sample : G4503-03
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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-BF112115.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	3.621	139	143	147	rBV	36749	90195	1.40%	0.190%
2	3.816	155	160	163	rBV2	45869	105904	1.64%	0.224%
3	4.056	176	181	186	rBV	130826	245848	3.80%	0.519%
4	4.181	188	192	196	rVB	67678	125328	1.94%	0.265%
5	4.650	231	233	235	rVB	66277	88432	1.37%	0.187%
6	4.730	235	240	248	rBV	736216	1231495	19.06%	2.601%
7	4.936	256	258	260	rBV2	73897	99483	1.54%	0.210%
8	5.199	279	281	290	rVV	1752562	2530238	39.16%	5.344%
9	5.324	290	292	295	rVV	61257	102055	1.58%	0.216%
10	5.370	295	296	298	rVV2	77045	103895	1.61%	0.219%
11	5.416	298	300	305	rVB2	55458	118893	1.84%	0.251%
12	5.599	311	316	318	rBV2	91401	180699	2.80%	0.382%
13	5.736	326	328	331	rBV3	109068	139315	2.16%	0.294%
14	5.839	335	337	341	rVB2	91805	129147	2.00%	0.273%
15	6.204	367	369	372	rBV	99346	113836	1.76%	0.240%
16	6.273	373	375	379	rBV	1654687	1609833	24.91%	3.400%
17	6.387	382	385	387	rBV	4091314	4634267	71.72%	9.788%
18	6.605	402	404	407	rBV	1014513	1071126	16.58%	2.262%
19	6.696	411	412	416	rVB	92341	74561	1.15%	0.157%
20	6.765	416	418	421	rBV	4341874	4149045	64.21%	8.763%
21	6.947	432	434	437	rVB2	57338	81679	1.26%	0.173%
22	7.039	437	442	444	rBV4	28648	65750	1.02%	0.139%
23	7.187	452	455	457	rBV	2944994	3980990	61.61%	8.408%
24	7.313	464	466	471	rVB3	60359	92320	1.43%	0.195%
25	7.896	515	517	520	rBV	1406549	1378657	21.34%	2.912%
26	8.982	609	612	615	rBV	6209996	6140063	95.02%	12.968%
27	9.382	645	647	649	rBV	314194	280566	4.34%	0.593%
28	9.599	664	666	668	rVB	83063	84947	1.31%	0.179%
29	9.645	668	670	673	rBV2	1464868	1570962	24.31%	3.318%
30	10.102	709	710	712	rVB	95709	67759	1.05%	0.143%
31	10.433	736	739	742	rBV2	3098130	3896854	60.31%	8.230%
32	10.571	750	751	754	rVB	99658	121233	1.88%	0.256%
33	10.822	769	773	774	rBV3	65857	88214	1.37%	0.186%
34	11.016	788	790	797	rVB2	91734	118218	1.83%	0.250%

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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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.119	797	799	802	rVV2	1271287	1547173	23.94%	3.268%
36	11.176	802	804	810	rVB2	42128	102837	1.59%	0.217%
37	11.439	825	827	830	rBV	57055	70323	1.09%	0.149%
38	11.599	838	841	846	rBV	32397	86353	1.34%	0.182%
39	11.679	846	848	853	rVV	703016	710422	10.99%	1.500%
40	11.828	859	861	864	rVB2	40797	65592	1.02%	0.139%
41	12.365	906	908	914	rBV4	46447	130389	2.02%	0.275%
42	12.468	914	917	922	rVV	366752	564533	8.74%	1.192%
43	12.719	936	939	941	rBV	5369842	6461682	100.00%	13.647%
44	13.622	1016	1018	1023	rBV2	86960	127630	1.98%	0.270%
45	13.748	1027	1029	1032	rBV	1546943	1483597	22.96%	3.133%
46	15.108	1145	1148	1151	rBV	953017	1086206	16.81%	2.294%

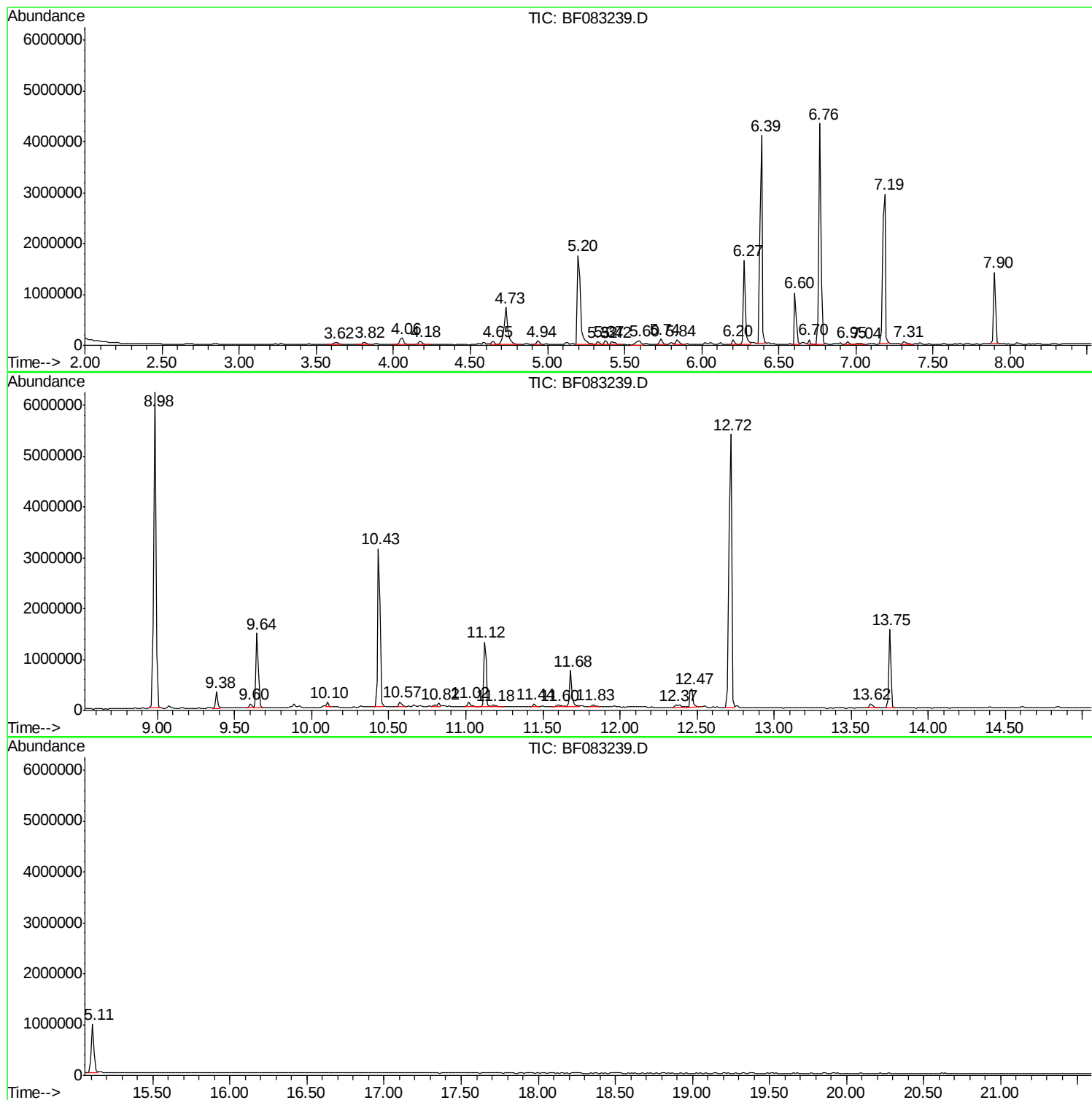
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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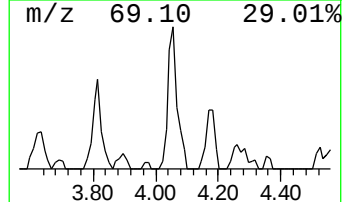
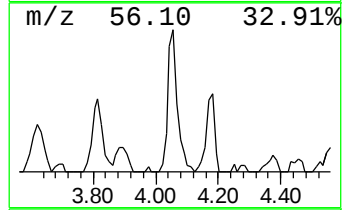
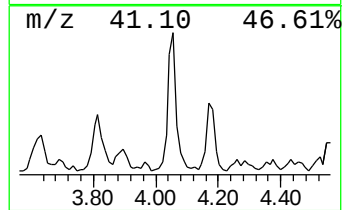
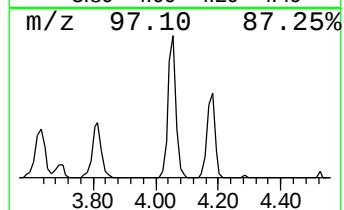
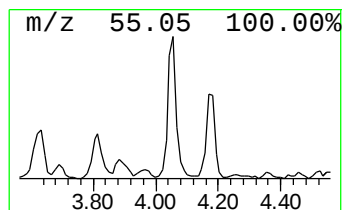
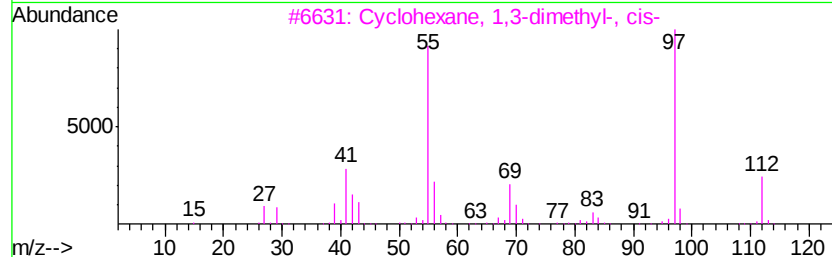
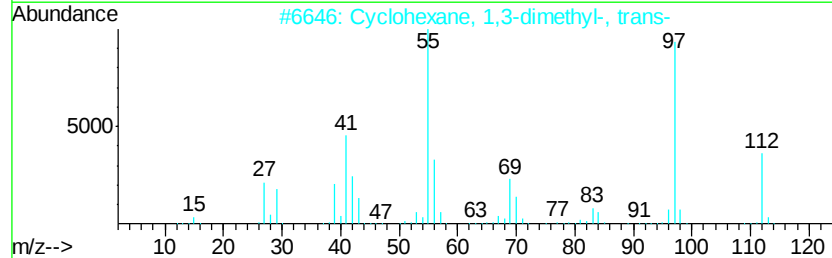
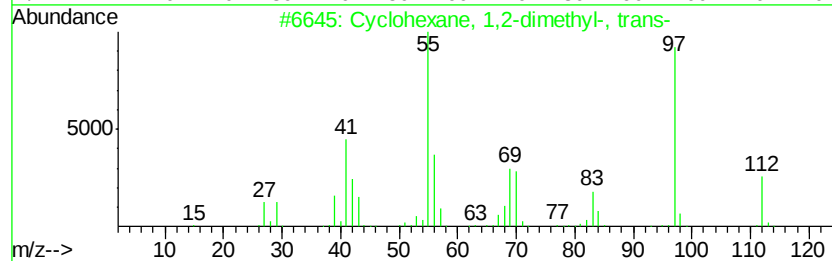
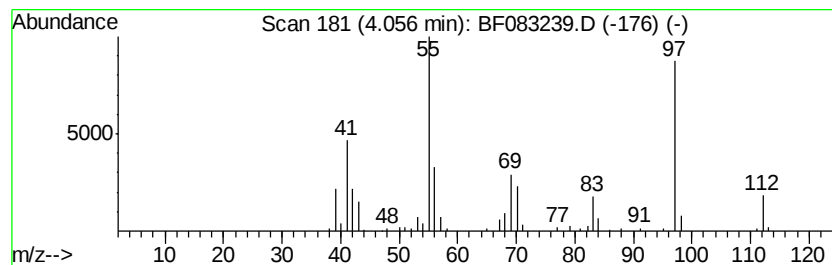
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.06	4.59 ng	245848	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
2		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	94
3		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87
4		Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	83
5		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	80



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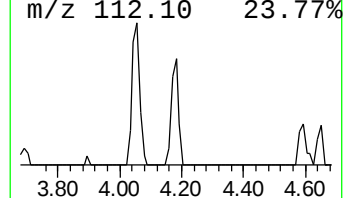
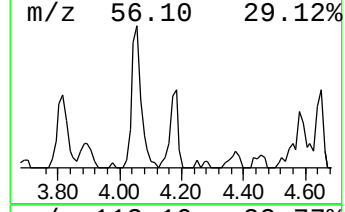
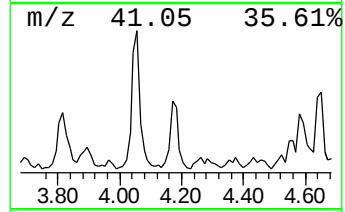
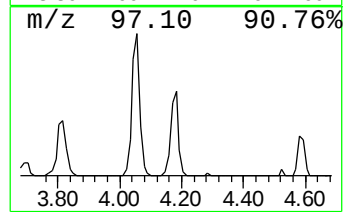
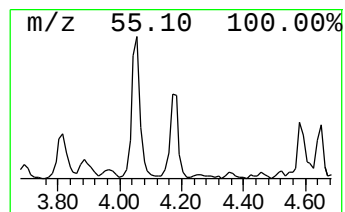
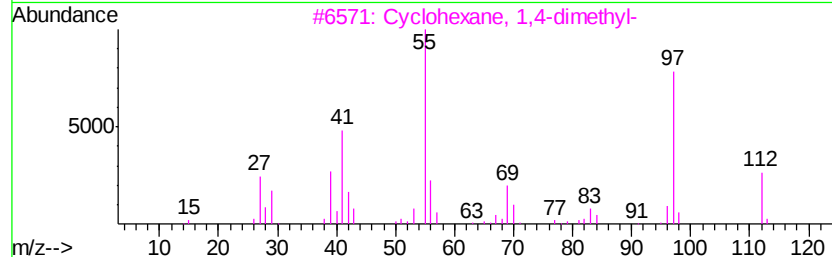
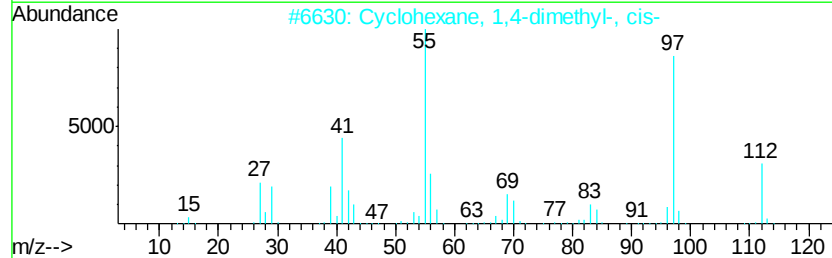
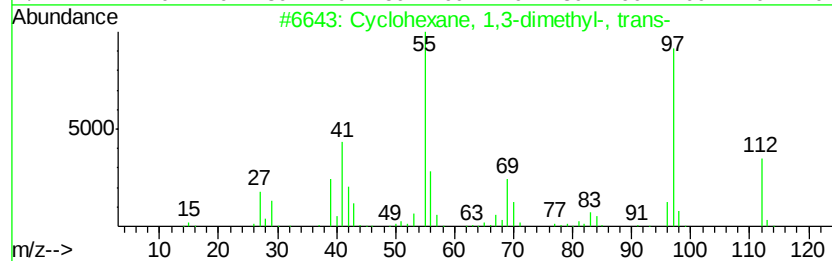
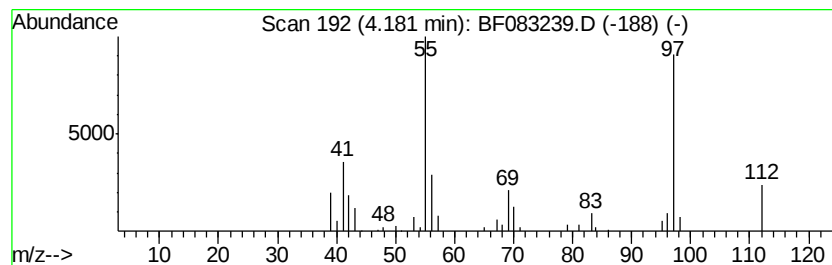
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Peak Number 2 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	2.34 ng	125328	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	94
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	91
3			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	91
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	90
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87



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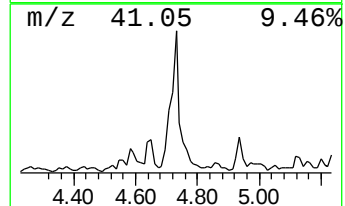
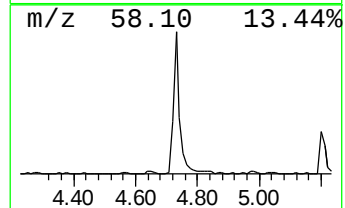
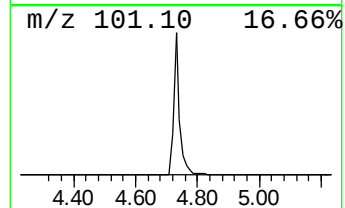
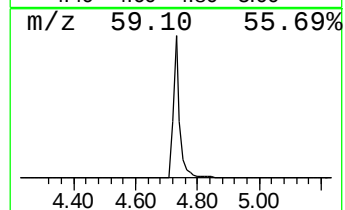
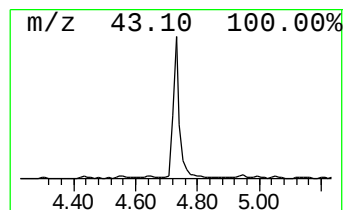
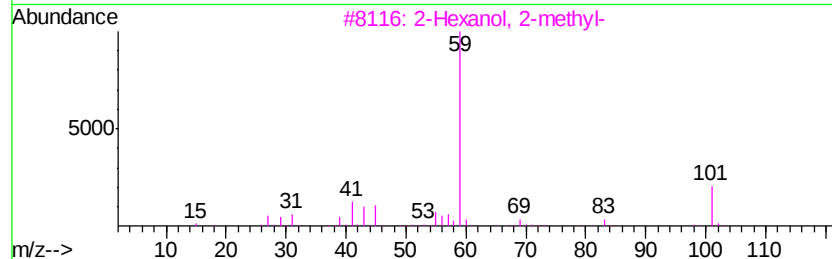
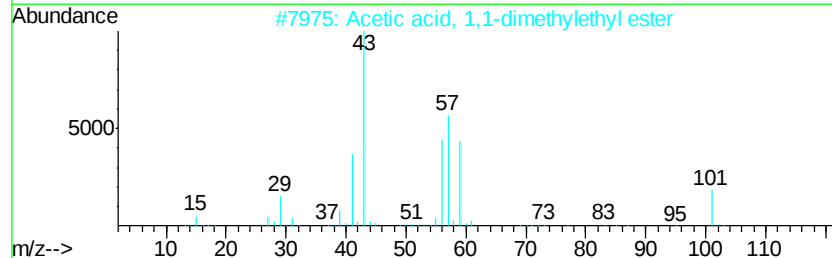
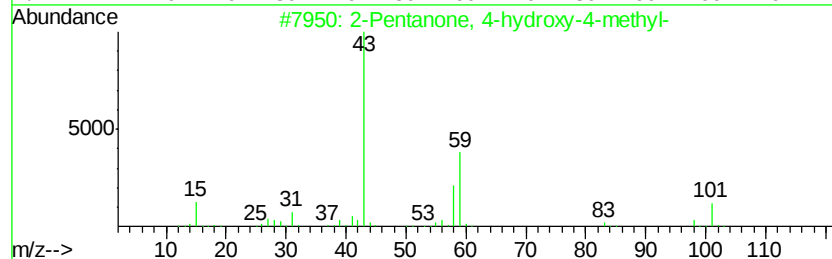
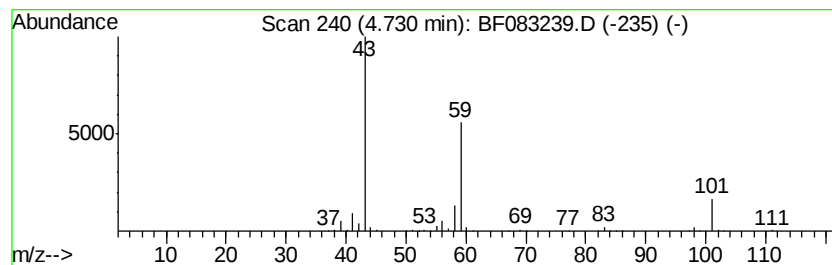
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	22.99 ng	1231500	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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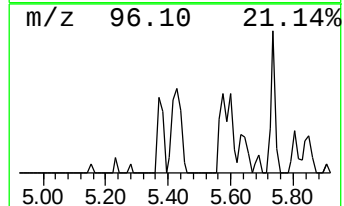
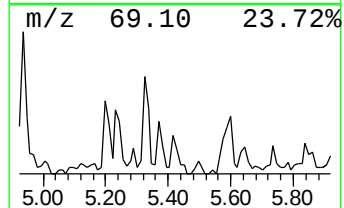
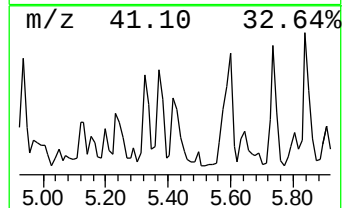
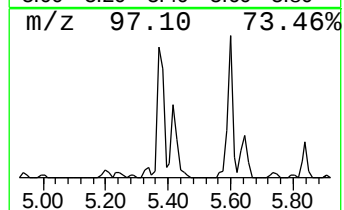
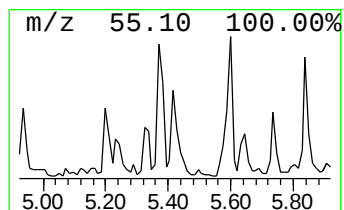
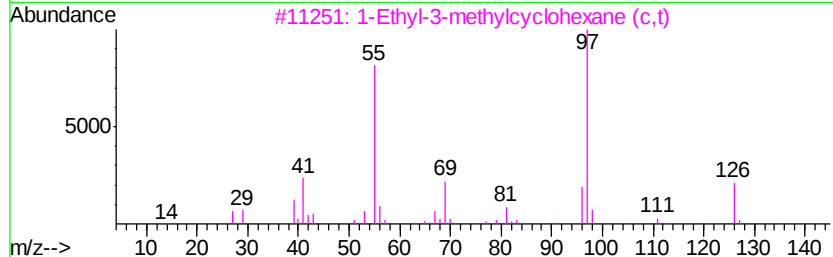
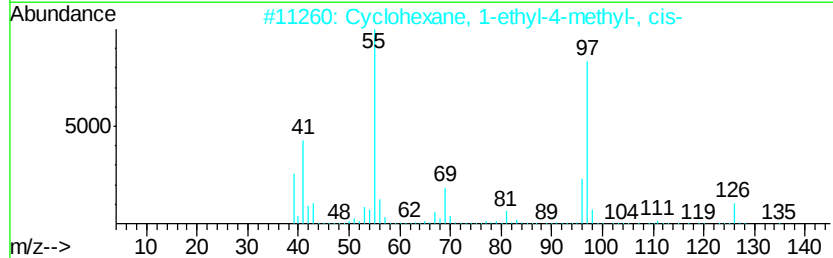
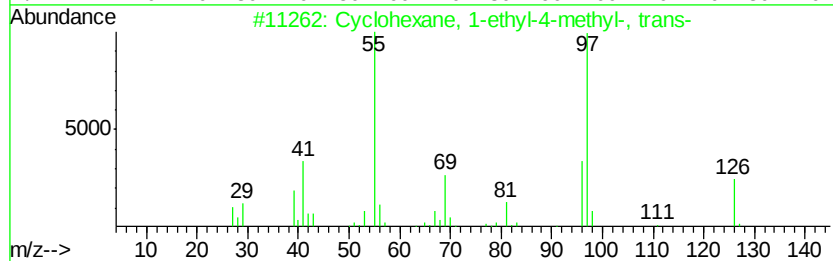
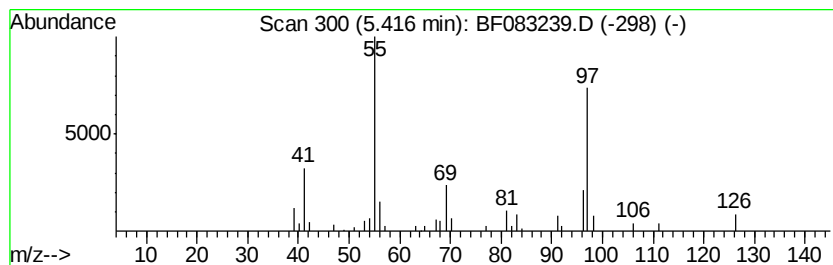
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.42	2.22 ng	118893	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	87
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
3		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	80
4		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	72
5		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	64



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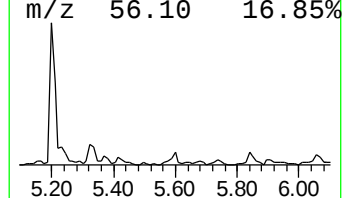
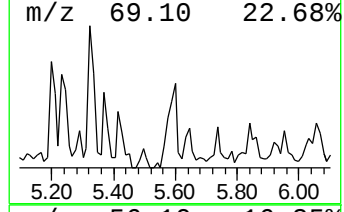
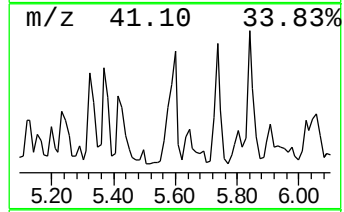
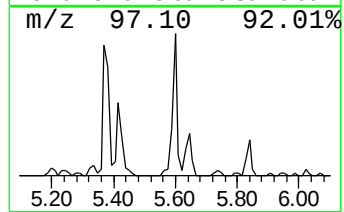
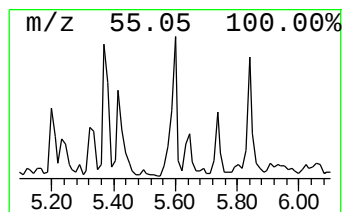
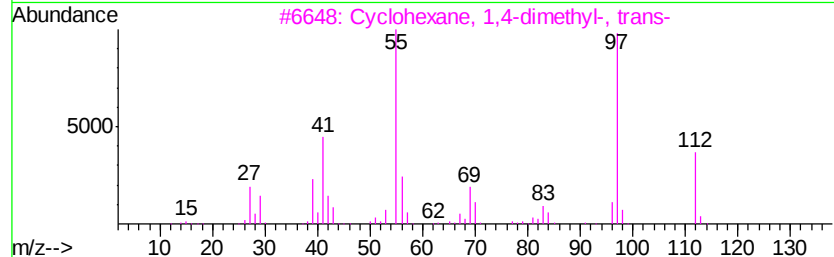
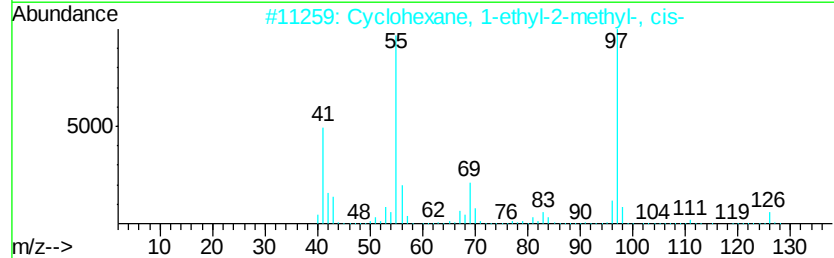
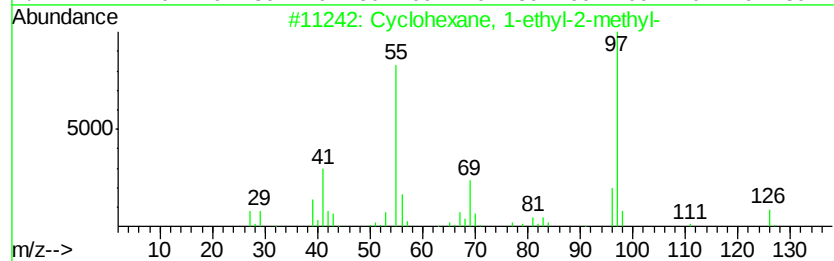
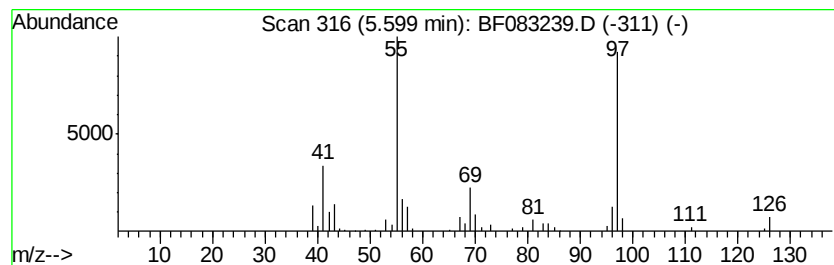
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	3.37 ng	180699	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	81
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	81
3		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	78
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	72
5		1,3-Dimethylcyclohexane,c&t	112	C8H16	000591-21-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
Acq On : 24 Nov 2015 16:19
Operator : UM/IZ
Sample : G4503-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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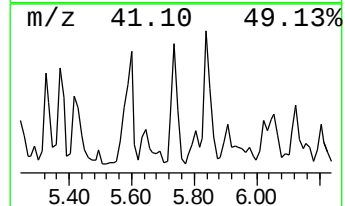
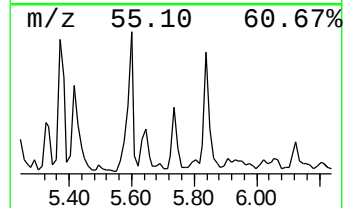
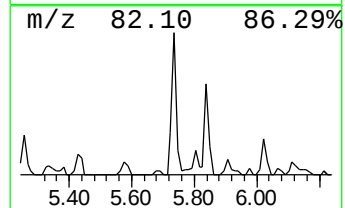
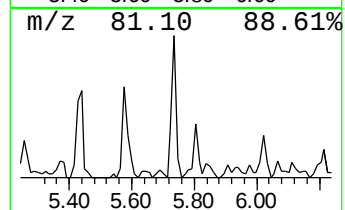
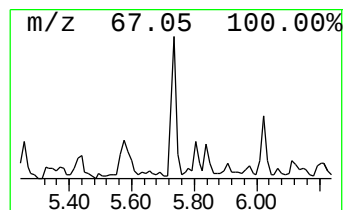
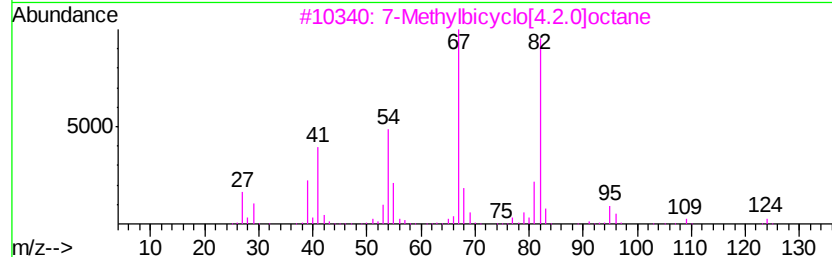
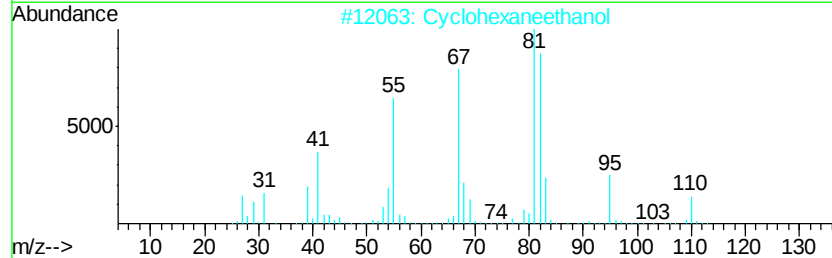
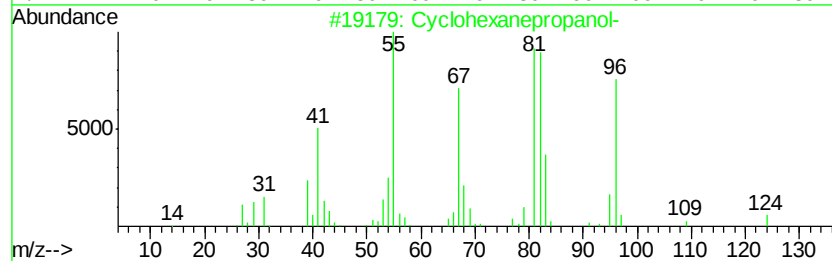
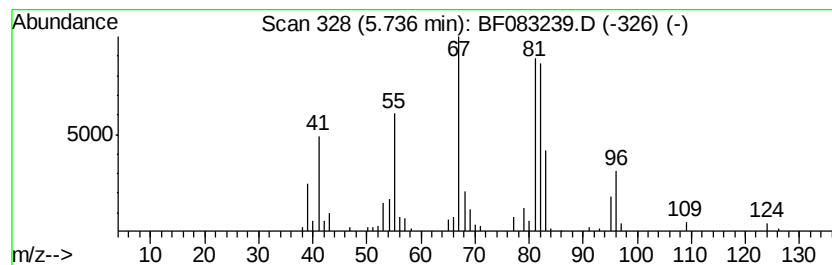
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexanepropanol- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	2.60 ng	139315	1,4-Dichlorobenzene-d4	6.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexanepropanol-	142	C9H18O	001124-63-6	90
2		Cyclohexaneethanol	128	C8H16O	004442-79-9	53
3		7-Methylbicyclo[4.2.0]octane	124	C9H16	1000210-90-2	49
4		Bicyclo[4.1.0]heptane	96	C7H12	000286-08-8	46
5		Cis-bicyclo[4.2.0]octane	110	C8H14	028282-35-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
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Sample : G4503-03
Misc :
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Instrument :
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ClientSampleId :
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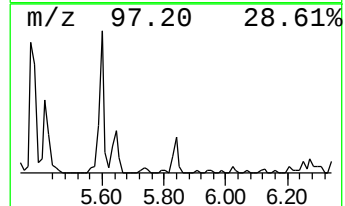
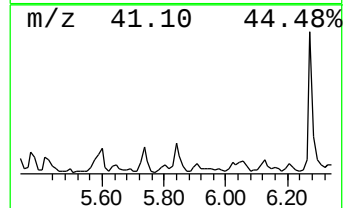
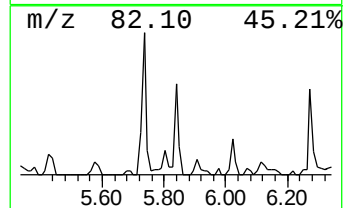
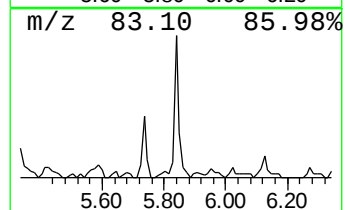
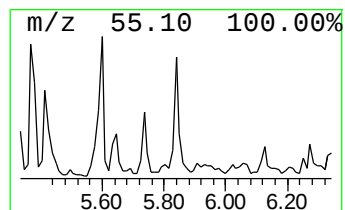
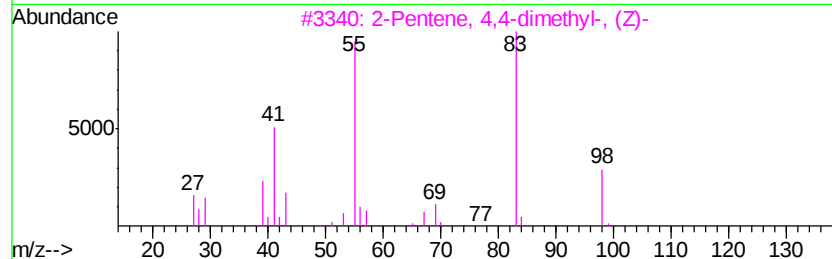
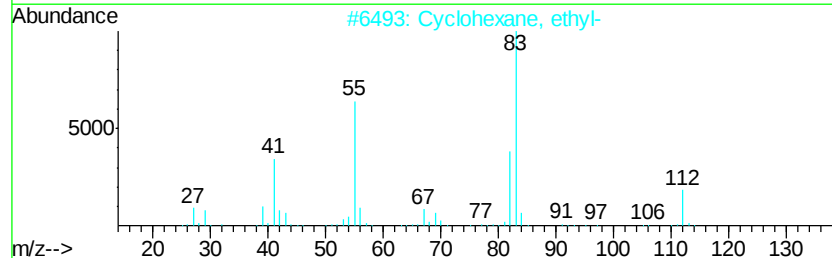
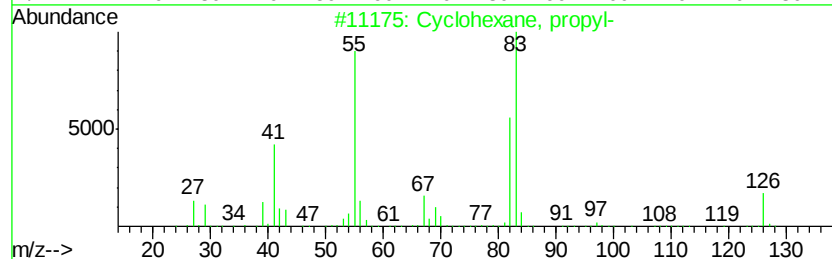
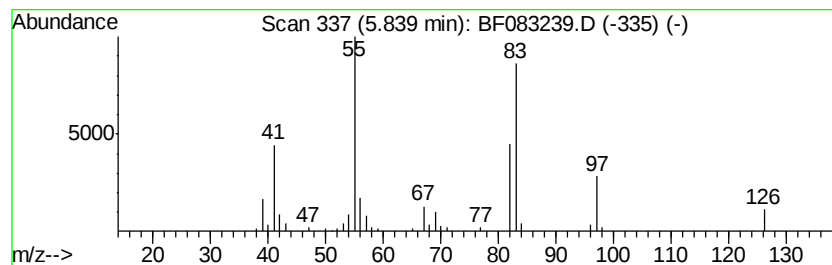
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexane, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	2.41 ng	129147	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	72
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	53
3		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	50
4		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	49
5		6-Dodecanol	186	C12H26O	006836-38-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
Acq On : 24 Nov 2015 16:19
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Sample : G4503-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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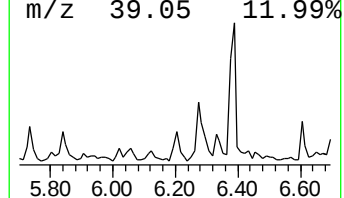
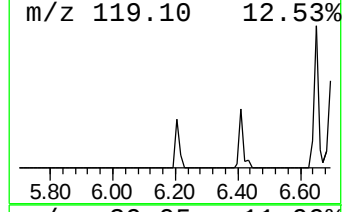
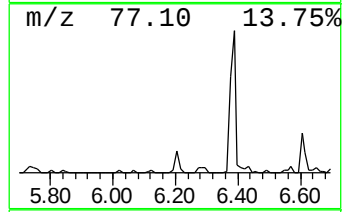
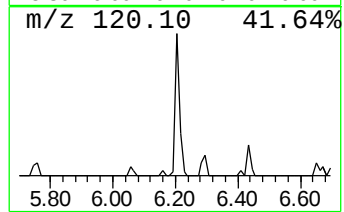
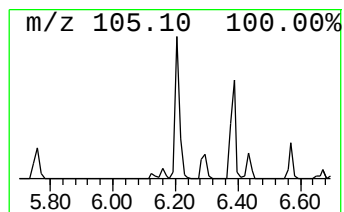
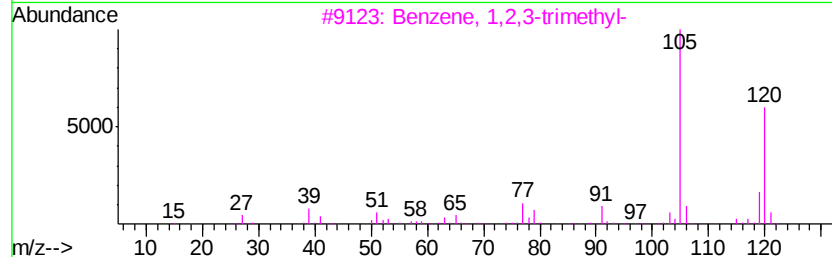
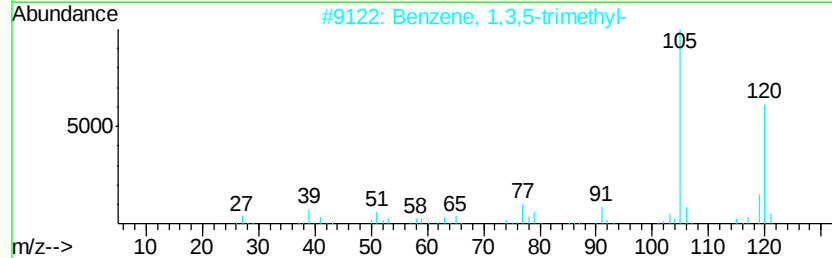
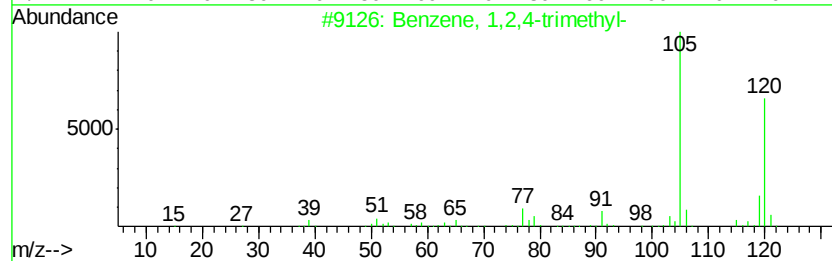
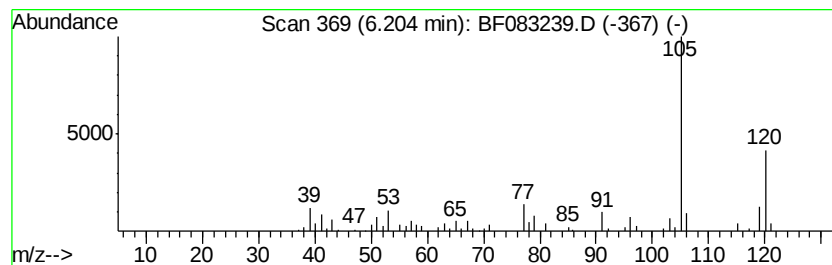
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1,2,4-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	2.13 ng	113836	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
2		Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
Acq On : 24 Nov 2015 16:19
Operator : UM/IZ
Sample : G4503-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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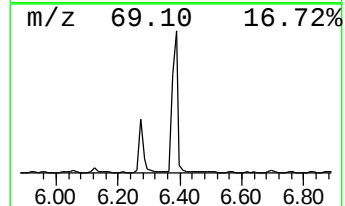
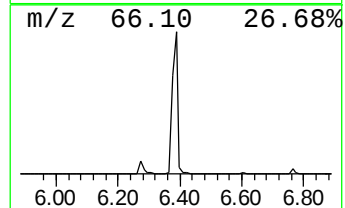
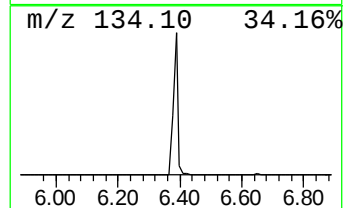
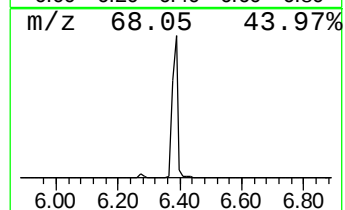
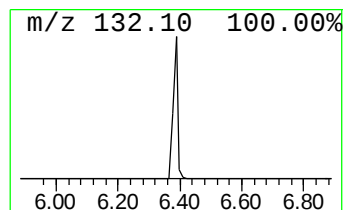
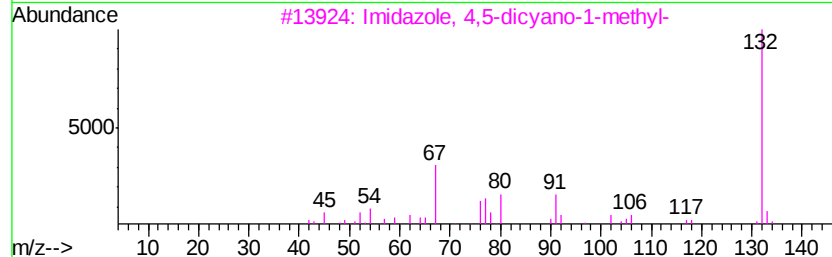
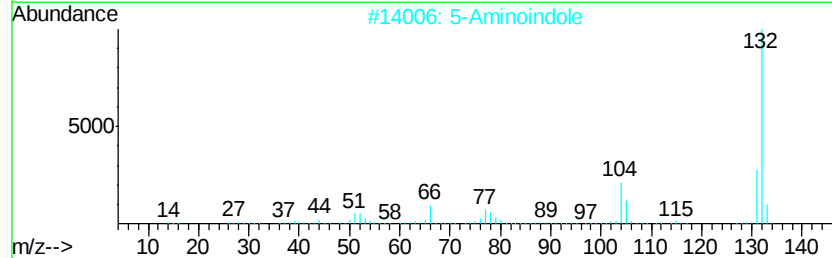
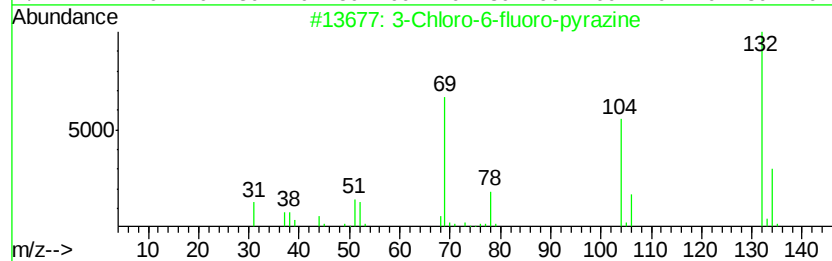
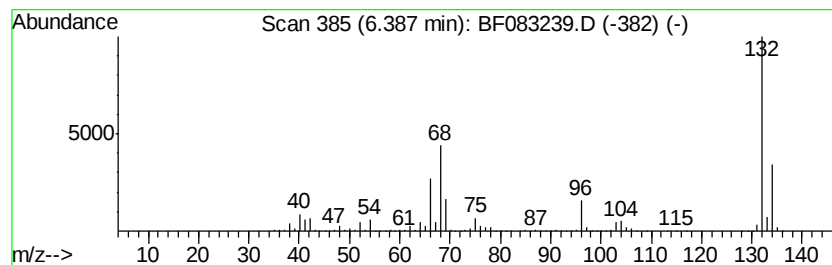
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	86.53 ng	4634270	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	9
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
Acq On : 24 Nov 2015 16:19
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Sample : G4503-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

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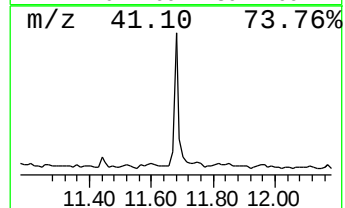
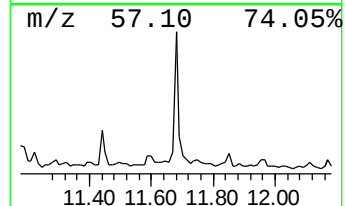
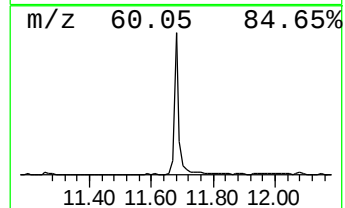
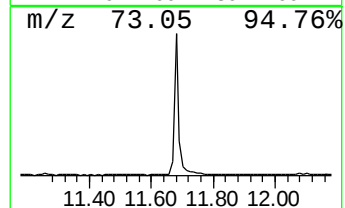
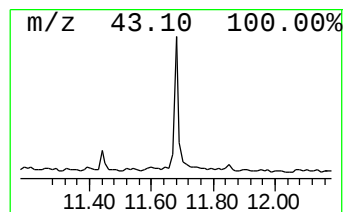
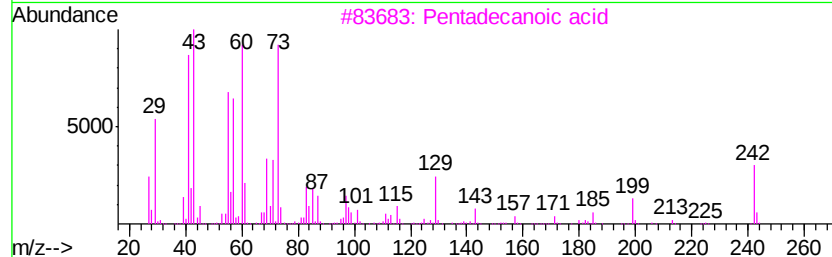
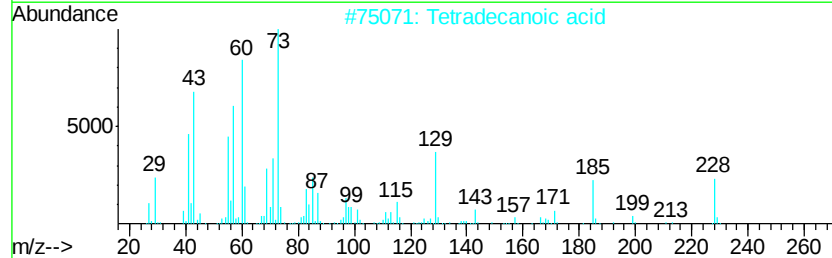
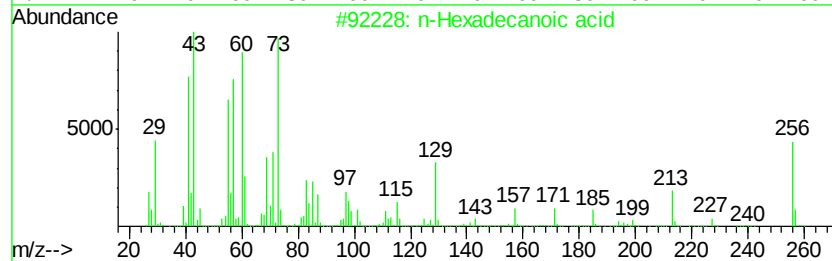
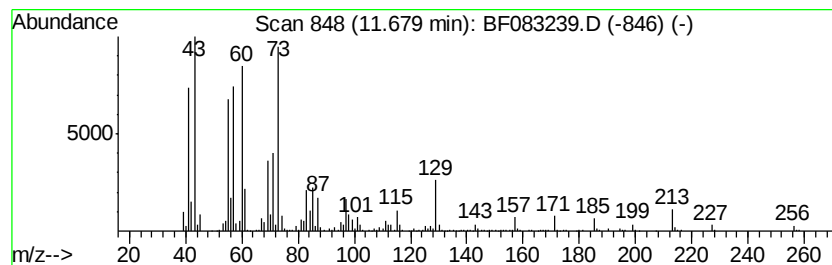
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	9.18 ng	710422	Phenanthrene-d10	11.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Undecanoic acid	186	C11H22O2	000112-37-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
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Sample : G4503-03
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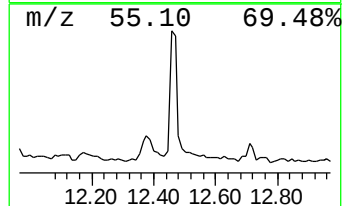
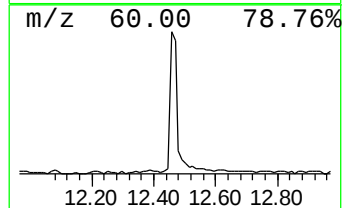
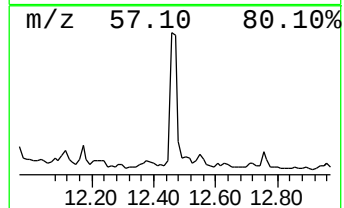
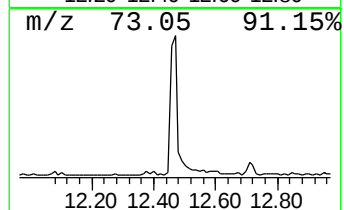
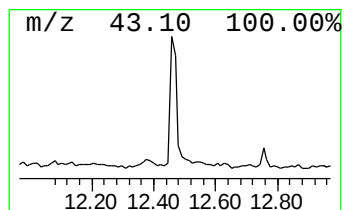
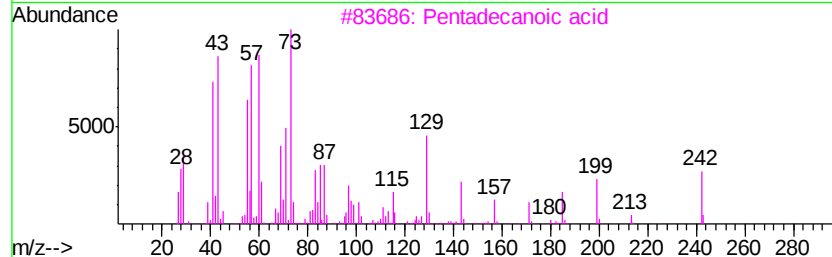
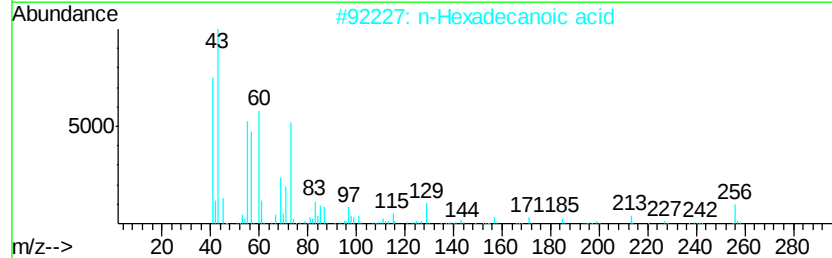
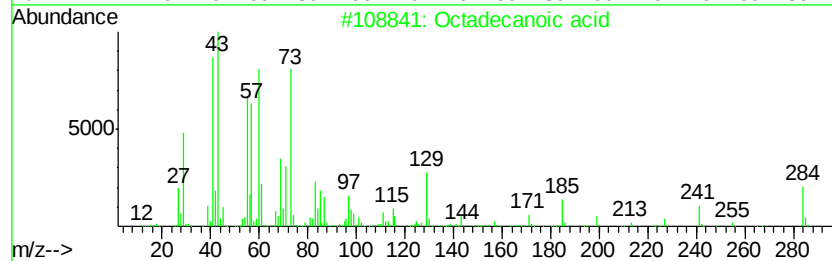
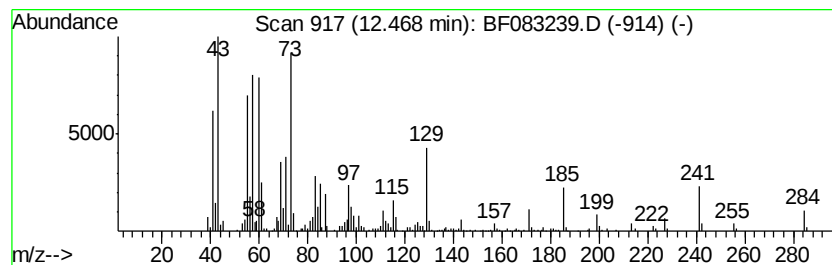
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.47	7.61 ng	564533	Chrysene-d12		13.75
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112415\
Data File : BF083239.D
Acq On : 24 Nov 2015 16:19
Operator : UM/IZ
Sample : G4503-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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
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Cyclohexane, 1,3-...	4.18	2.3	ng	125328	1	6.60	1071130	20.0
2-Pentanone, 4-hy...	4.73	23.0	ng	1231500	1	6.60	1071130	20.0
Cyclohexane, 1-et...	5.42	2.2	ng	118893	1	6.60	1071130	20.0
Cyclohexane, 1-et...	5.60	3.4	ng	180699	1	6.60	1071130	20.0
Cyclohexanepropanol-	5.74	2.6	ng	139315	1	6.60	1071130	20.0
Cyclohexane, propyl-	5.84	2.4	ng	129147	1	6.60	1071130	20.0
Benzene, 1,2,4-tr...	6.20	2.1	ng	113836	1	6.60	1071130	20.0
unknown6.39	6.39	86.5	ng	4634270	1	6.60	1071130	20.0
n-Hexadecanoic acid	11.68	9.2	ng	710422	4	11.12	1547170	20.0
Octadecanoic acid	12.47	7.6	ng	564533	5	13.75	1483600	20.0