

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
 Data File : BF087197.D
 Acq On : 19 May 2016 20:06
 Operator : UM/SJ
 Sample : H3138-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF051716.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	1.712	9	11	39	rVB	2271406	4844000	99.05%	11.732%
2	4.524	252	257	259	rBV	51793	87166	1.78%	0.211%
3	4.661	266	269	270	rBV	51320	76643	1.57%	0.186%
4	4.696	270	272	275	rVV2	115954	254304	5.20%	0.616%
5	4.753	275	277	286	rVV2	92368	227365	4.65%	0.551%
6	4.936	289	293	295	rVV2	44461	82732	1.69%	0.200%
7	5.027	297	301	304	rBV2	27712	61943	1.27%	0.150%
8	5.141	309	311	331	rBV	1121237	2134697	43.65%	5.170%
9	5.884	373	376	386	rVB	61314	83966	1.72%	0.203%
10	6.181	398	402	404	rBV	31096	57385	1.17%	0.139%
11	6.227	404	406	411	rVV2	980947	1662739	34.00%	4.027%
12	6.296	411	412	414	rVV	270096	268100	5.48%	0.649%
13	6.342	414	416	418	rVV	2722576	3558661	72.77%	8.619%
14	6.399	420	421	422	rVV	142929	192791	3.94%	0.467%
15	6.422	422	423	428	rVB	1017571	857221	17.53%	2.076%
16	6.559	433	435	438	rBV	1127647	1249735	25.55%	3.027%
17	6.604	438	439	440	rVV	252446	210411	4.30%	0.510%
18	6.639	440	442	445	rVB2	241665	476777	9.75%	1.155%
19	6.719	446	449	452	rBV	3333604	3079990	62.98%	7.459%
20	7.142	484	486	495	rBV	2789534	2914719	59.60%	7.059%
21	7.850	546	548	551	rBV	1208364	1174250	24.01%	2.844%
22	8.147	572	574	577	rBV	42021	51894	1.06%	0.126%
23	8.422	595	598	599	rBV	49366	52312	1.07%	0.127%
24	8.776	627	629	631	rBV	79195	90461	1.85%	0.219%
25	8.936	640	643	645	rBV	4843945	4890379	100.00%	11.844%
26	9.336	676	678	679	rBV	70285	65332	1.34%	0.158%
27	9.370	679	681	684	rVB	59057	76560	1.57%	0.185%
28	9.428	684	686	687	rBV	86410	83273	1.70%	0.202%
29	9.542	693	696	698	rBV	128854	142832	2.92%	0.346%
30	9.599	698	701	704	rBV2	1705412	2011892	41.14%	4.873%
31	10.388	767	770	773	rBV2	2490776	2923026	59.77%	7.079%
32	10.513	780	781	786	rVB2	53193	62427	1.28%	0.151%
33	10.765	799	803	805	rVB	30972	69231	1.42%	0.168%
34	10.959	818	820	822	rBV2	55837	53336	1.09%	0.129%

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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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.073	828	830	833	rBV	1268535	1222236	24.99%	2.960%
36	11.473	861	865	867	rVB2	212495	203361	4.16%	0.493%
37	11.633	875	879	884	rVB4	50796	133937	2.74%	0.324%
38	12.662	966	969	971	rBV	3822250	3810786	77.92%	9.229%
39	13.577	1047	1049	1057	rBV	50384	125892	2.57%	0.305%
40	13.702	1057	1060	1063	rBV	969168	917340	18.76%	2.222%
41	15.051	1175	1178	1181	rBV	640965	748362	15.30%	1.812%

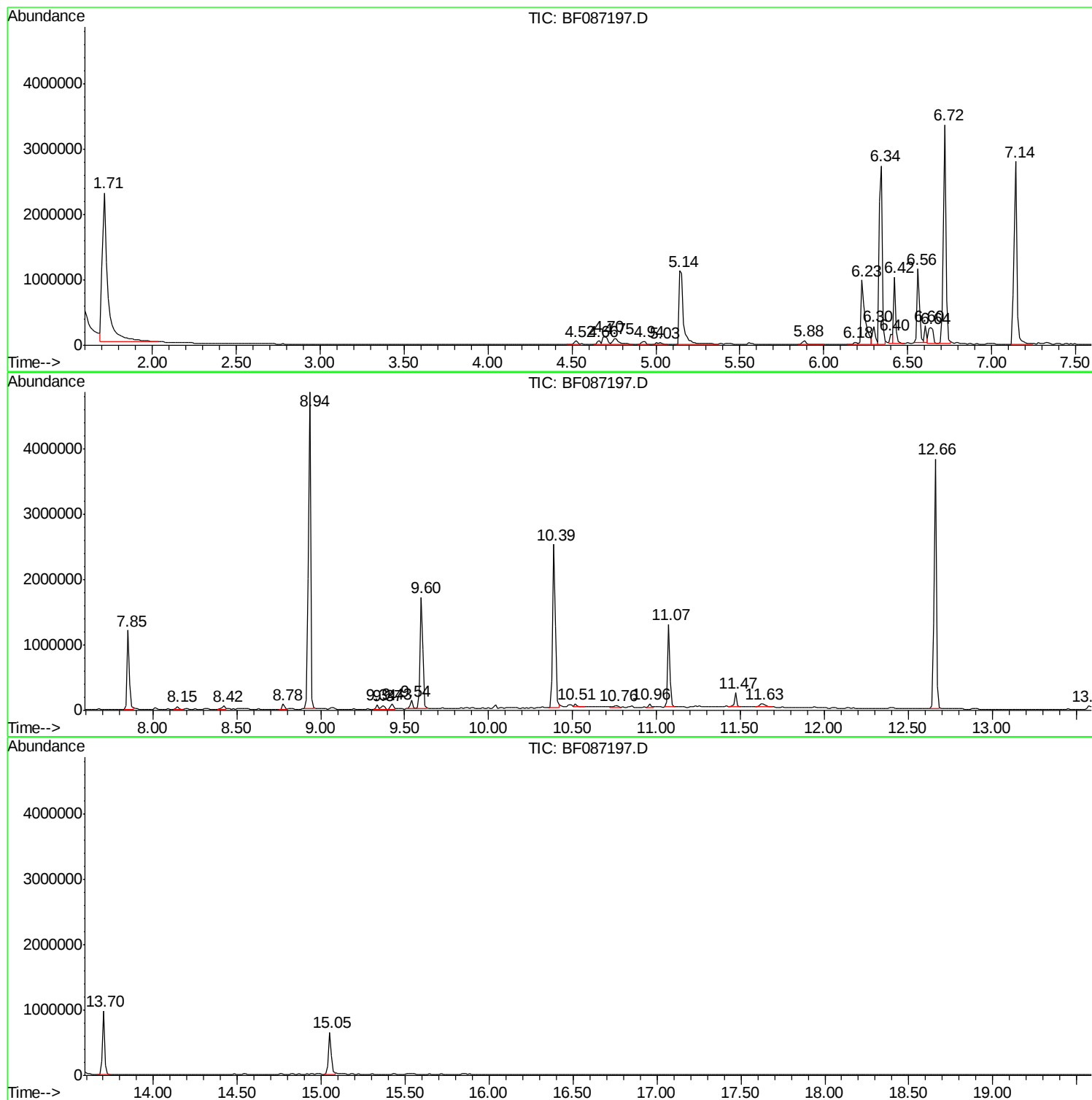
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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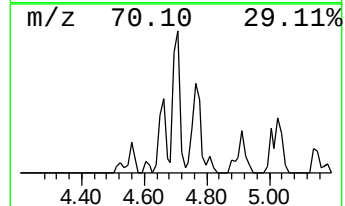
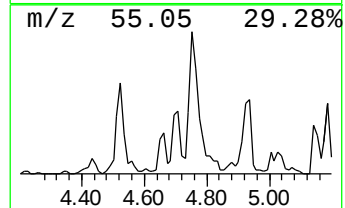
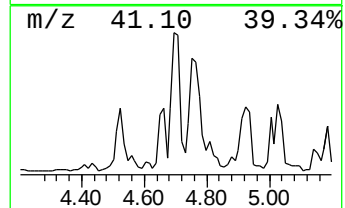
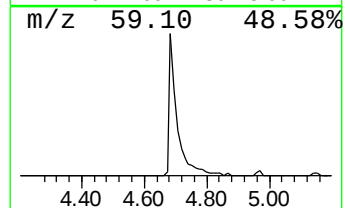
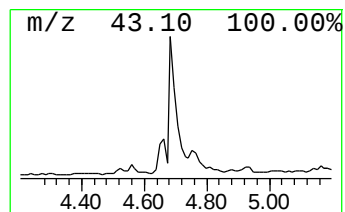
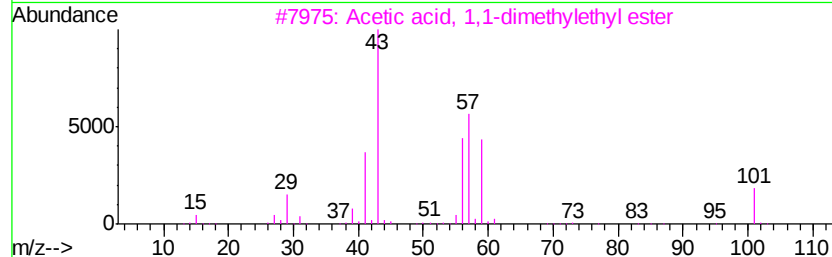
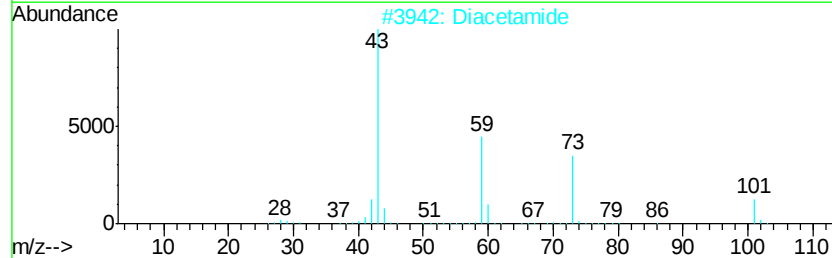
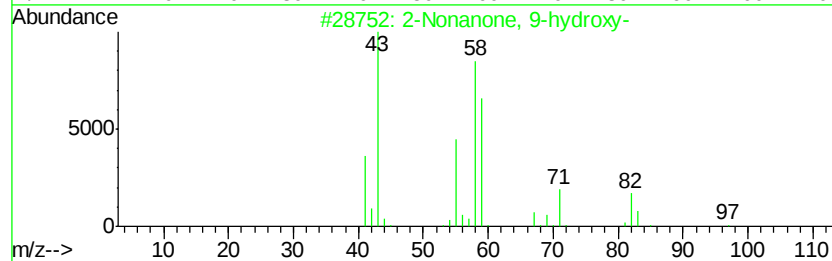
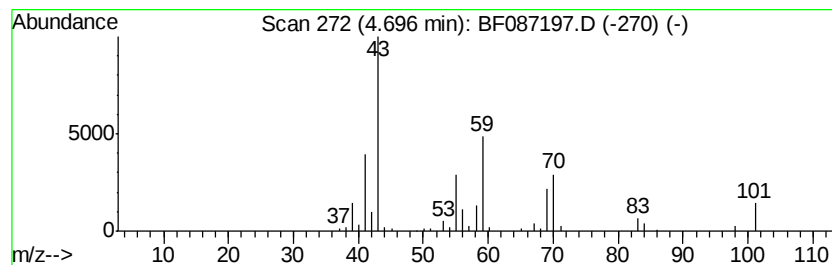
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.70 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	4.07 ng	254304	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	32
2			Diacetamide	101	C4H7NO2	000625-77-4	28
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	17
5			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12



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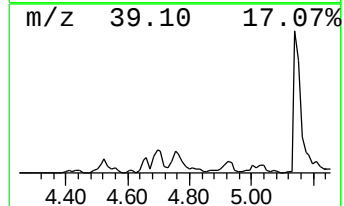
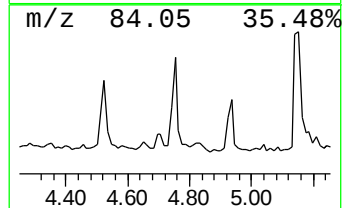
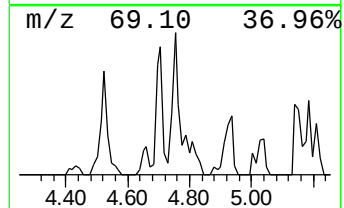
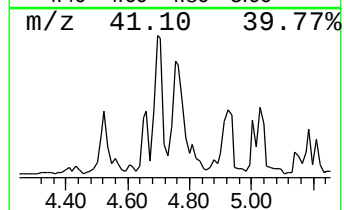
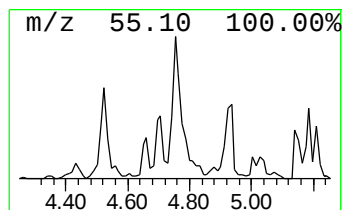
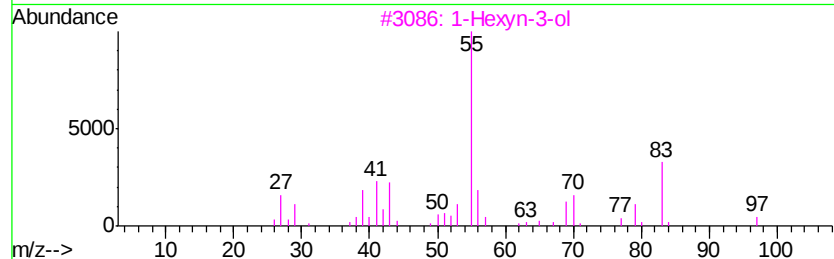
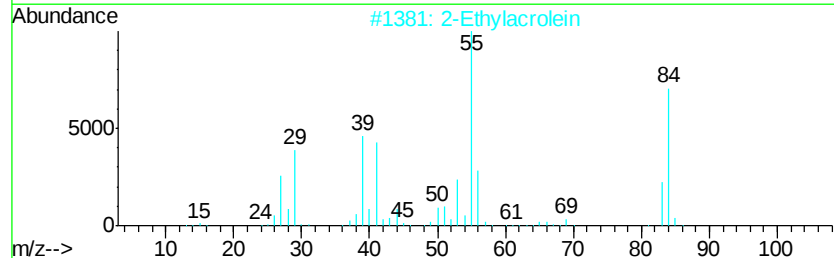
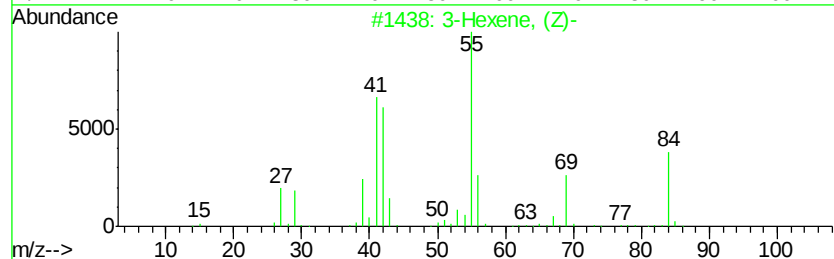
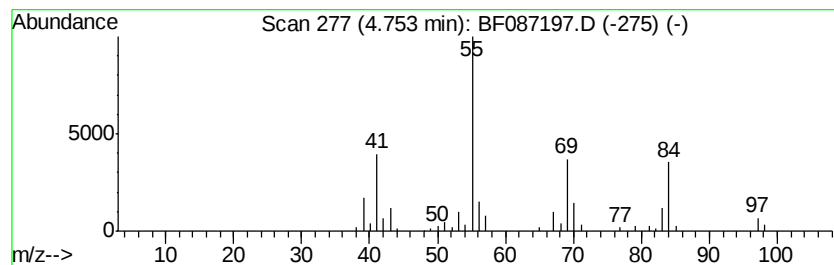
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown4.75 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	3.64 ng	227365	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexene, (Z)-	84	C6H12	007642-09-3	47
2			2-Ethylacrolein	84	C5H8O	000922-63-4	47
3			1-Hexyn-3-ol	98	C6H10O	000105-31-7	38
4			2-Pentenal, (E)-	84	C5H8O	001576-87-0	38
5			3-Hexene, (E)-	84	C6H12	013269-52-8	38



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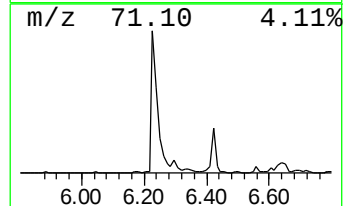
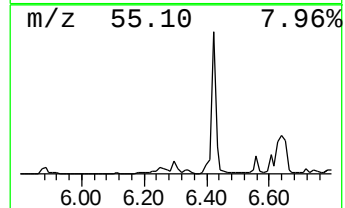
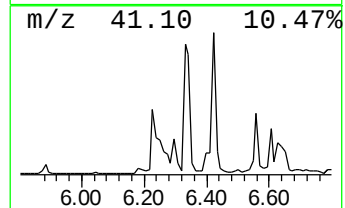
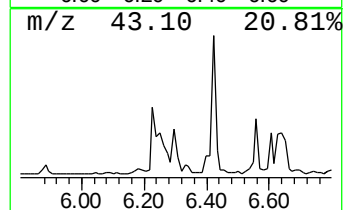
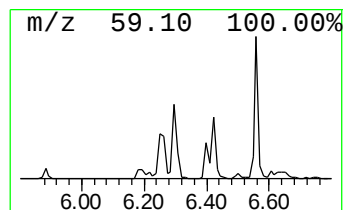
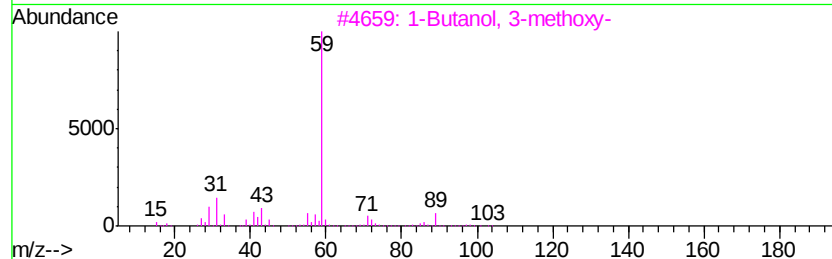
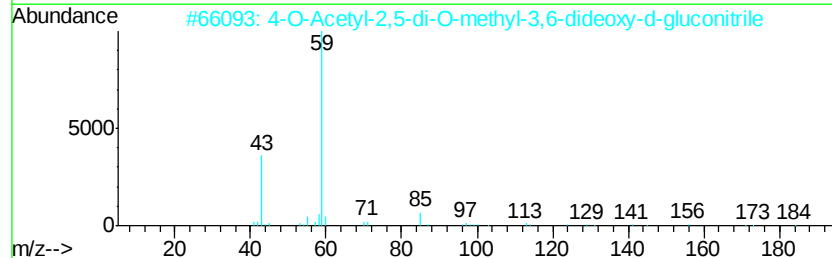
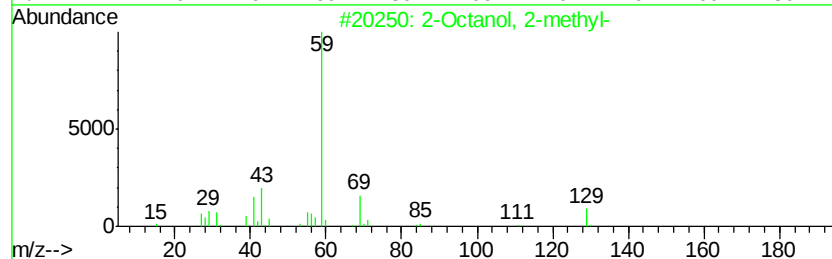
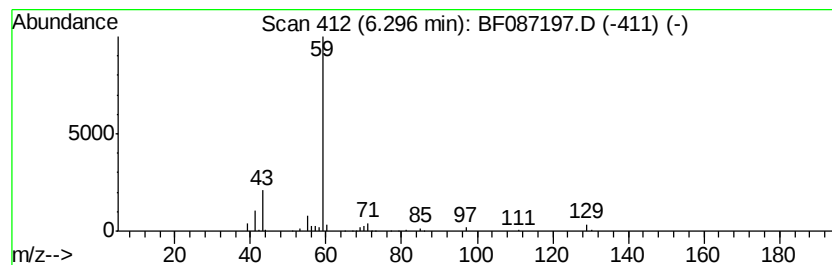
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	4.29 ng	268100	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	64
2		4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1000101-80-3	40
3		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	40
4		Amylene Hydrate	88	C5H12O	000075-85-4	39
5		2-Hydroxy-2,5-dimethyl-hept-6-en...	156	C9H16O2	1000192-55-8	39



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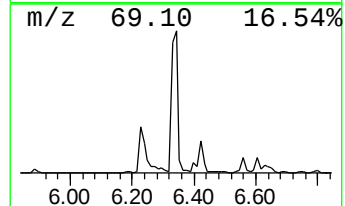
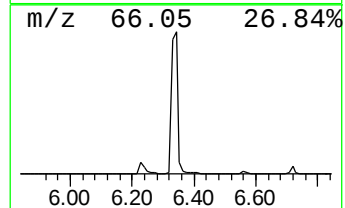
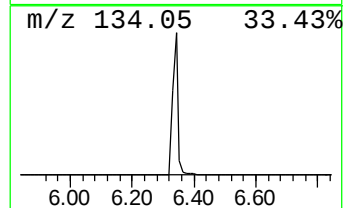
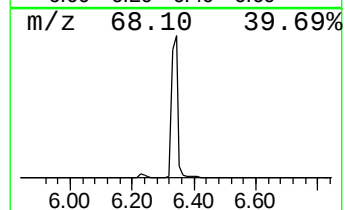
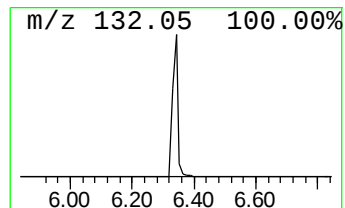
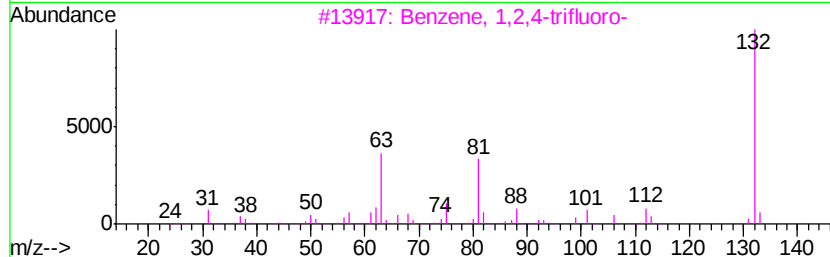
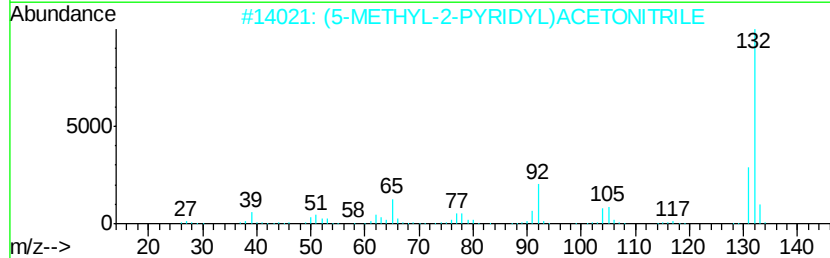
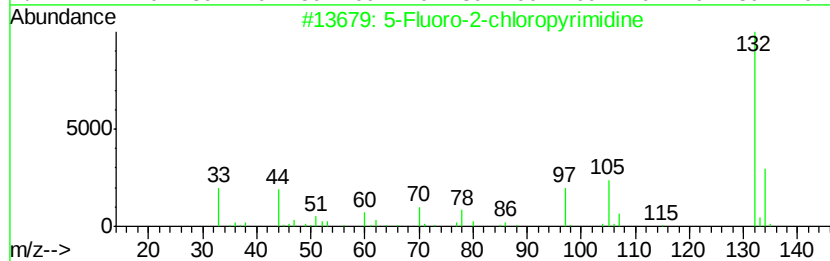
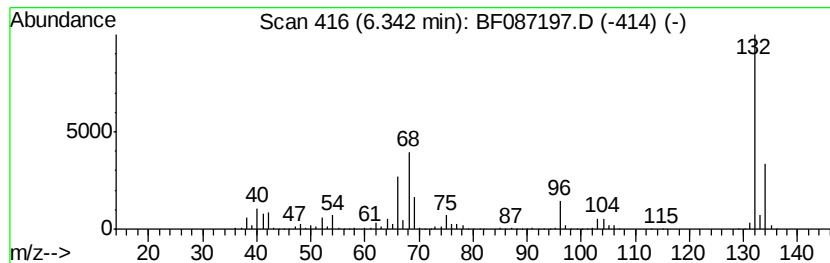
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	56.95 ng	3558660	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	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



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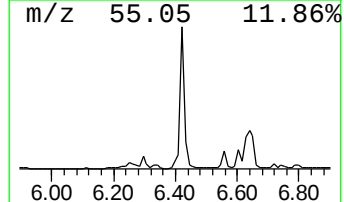
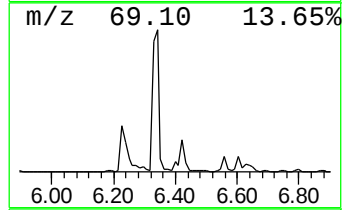
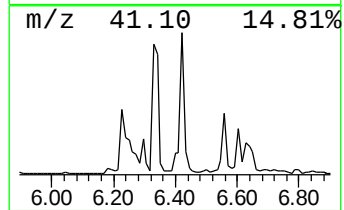
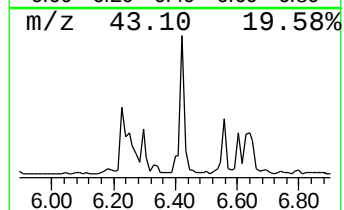
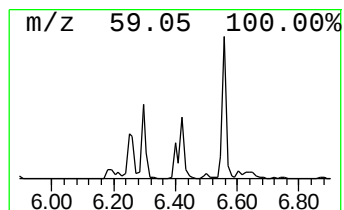
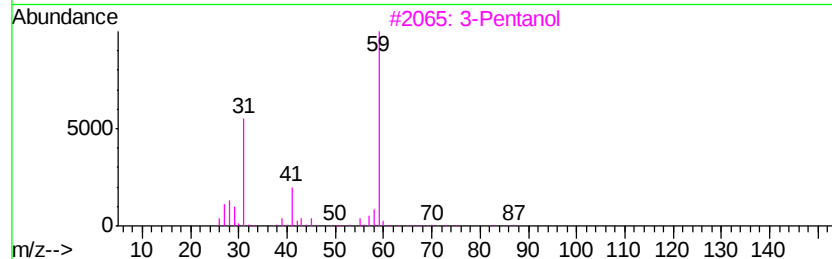
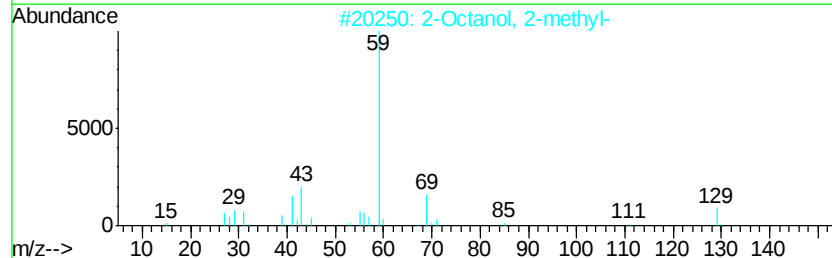
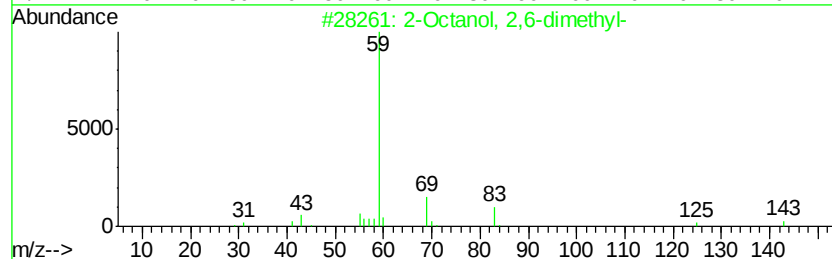
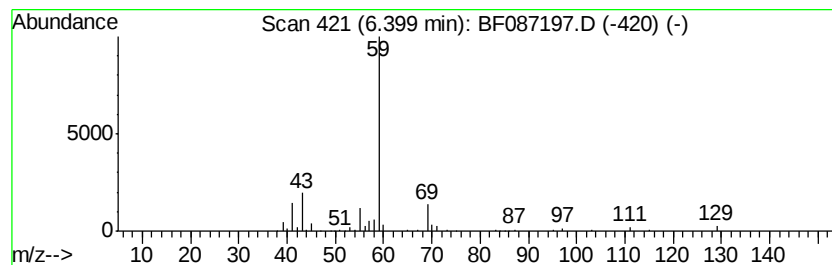
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Peak Number 6 2-Octanol, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	3.09 ng	192791	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	56
2			2-Octanol, 2-methyl-	144	C9H20O	000628-44-4	56
3			3-Pentanol	88	C5H12O	000584-02-1	50
4			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	39
5			Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
Data File : BF087197.D
Acq On : 19 May 2016 20:06
Operator : UM/SJ
Sample : H3138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

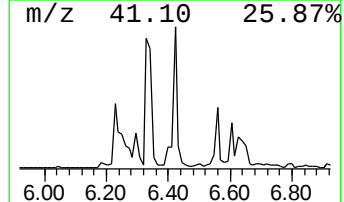
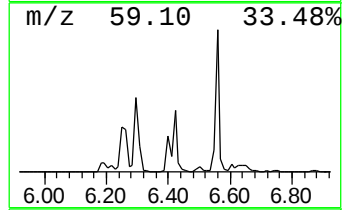
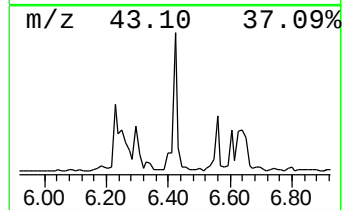
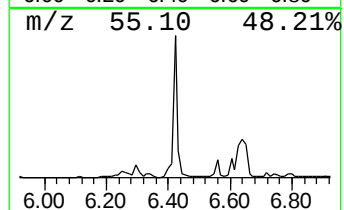
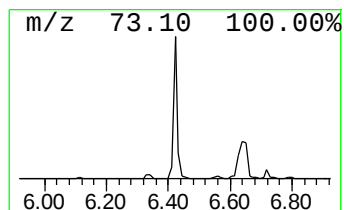
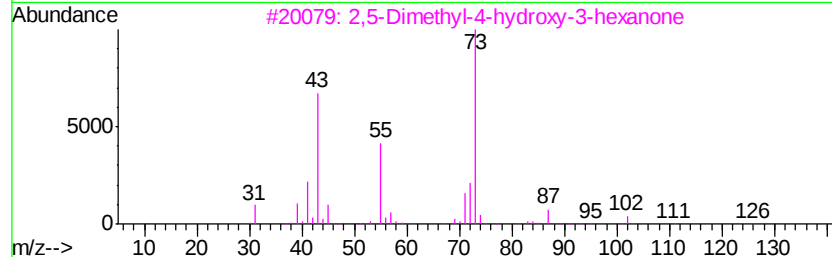
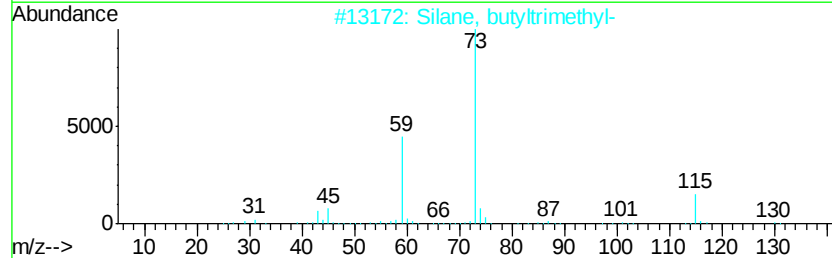
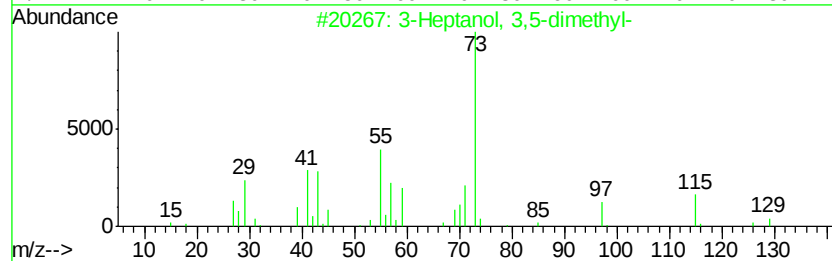
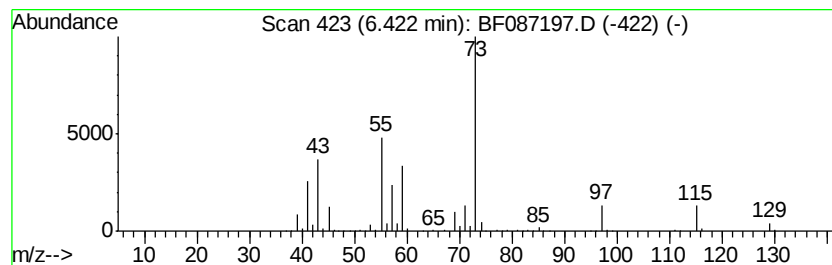
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Heptanol, 3,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	13.72 ng	857221	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	50
2			Silane, butyltrimethyl-	130	C7H18Si	001000-49-3	38
3			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	35
4			3-Octanol, 3-methyl-	144	C9H20O	005340-36-3	35
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
Data File : BF087197.D
Acq On : 19 May 2016 20:06
Operator : UM/SJ
Sample : H3138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

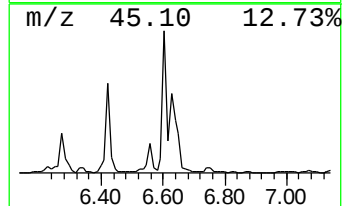
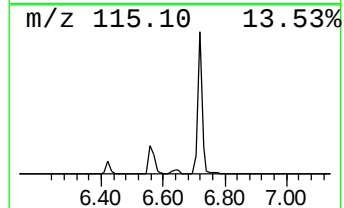
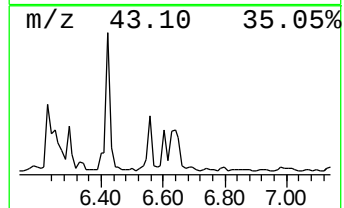
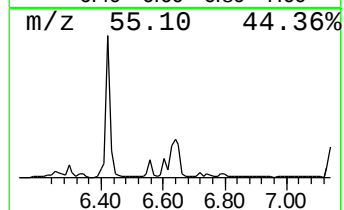
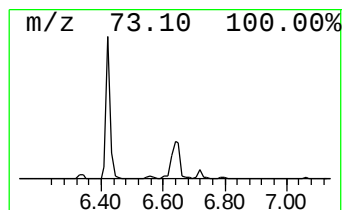
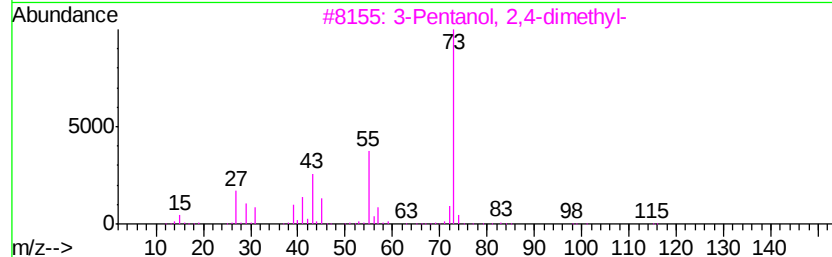
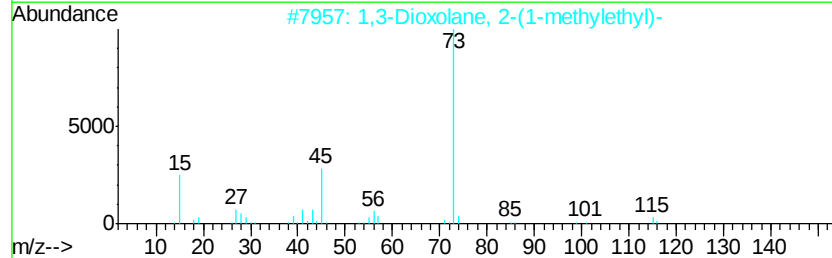
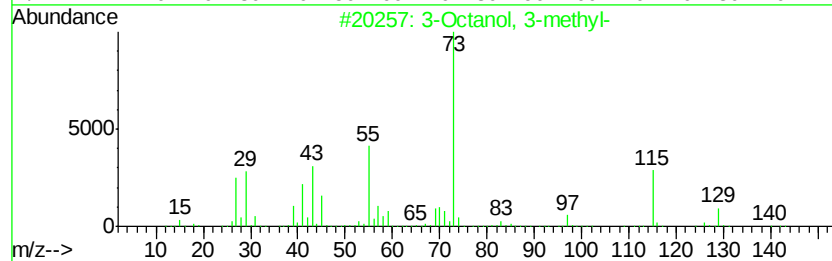
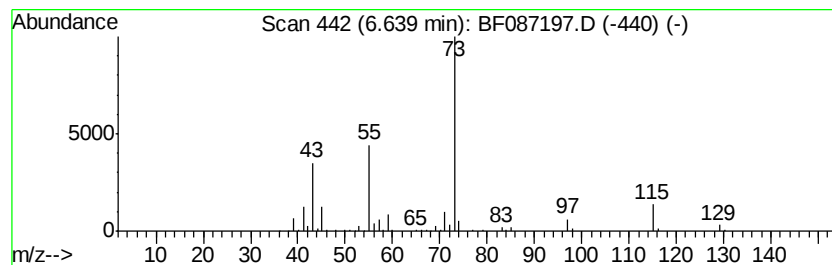
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown6.64 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	7.63 ng	476777	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octanol, 3-methyl-	144	C9H20O	005340-36-3	47
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	43
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
4		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	40
5		3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	36



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
Data File : BF087197.D
Acq On : 19 May 2016 20:06
Operator : UM/SJ
Sample : H3138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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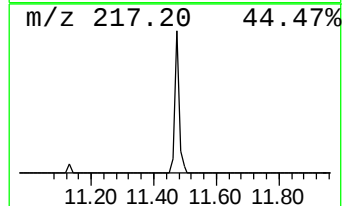
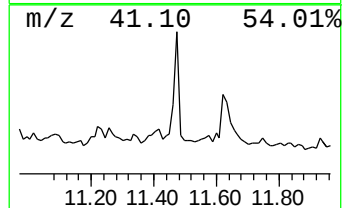
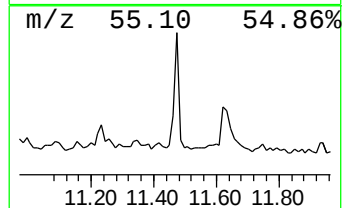
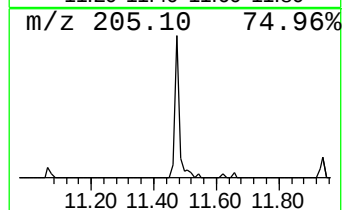
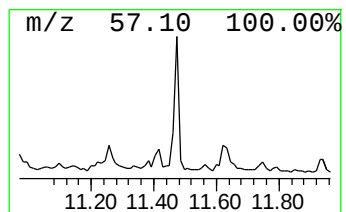
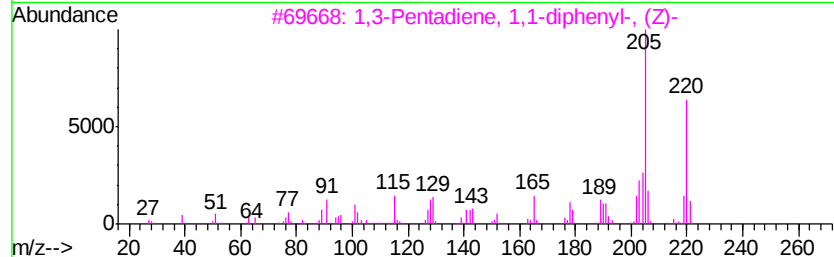
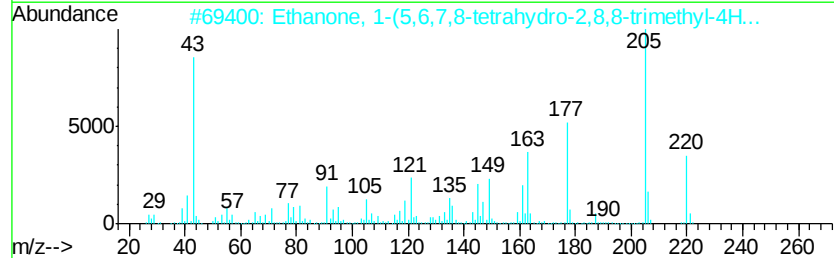
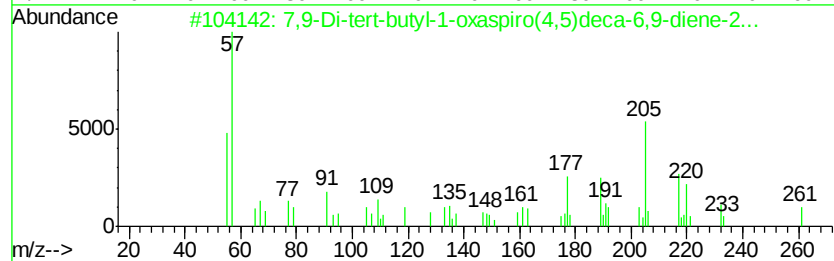
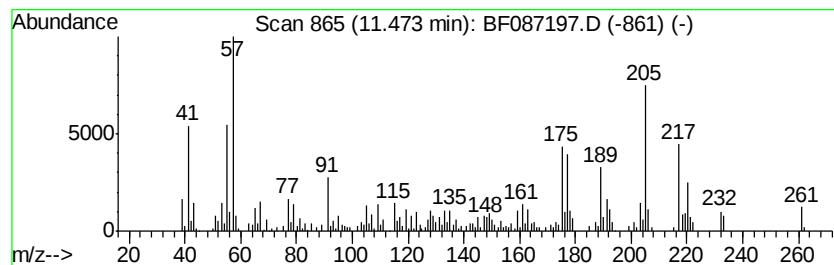
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	3.33 ng	203361	Phenanthrene-d10	11.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	92
2			Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3			1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	49
4			2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	45
5			Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
Data File : BF087197.D
Acq On : 19 May 2016 20:06
Operator : UM/SJ
Sample : H3138-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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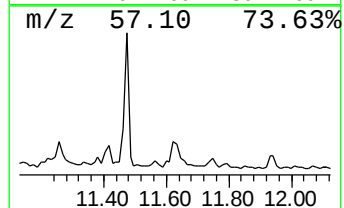
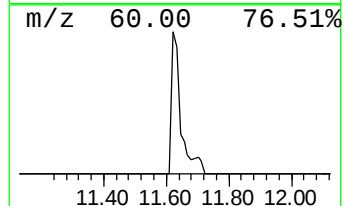
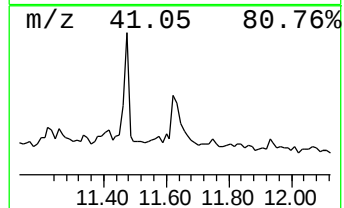
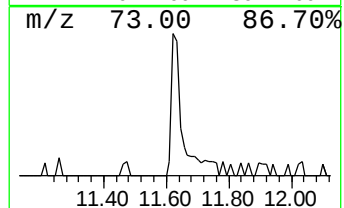
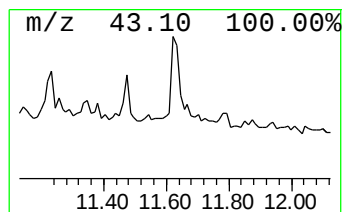
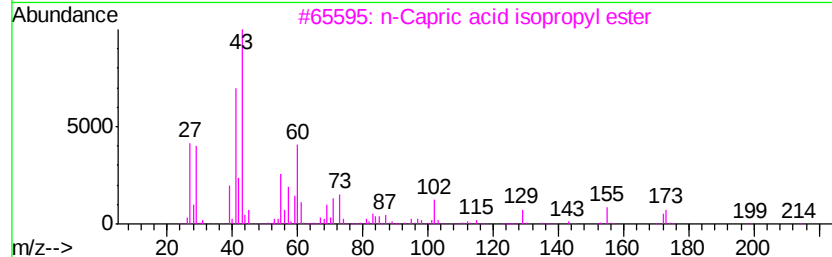
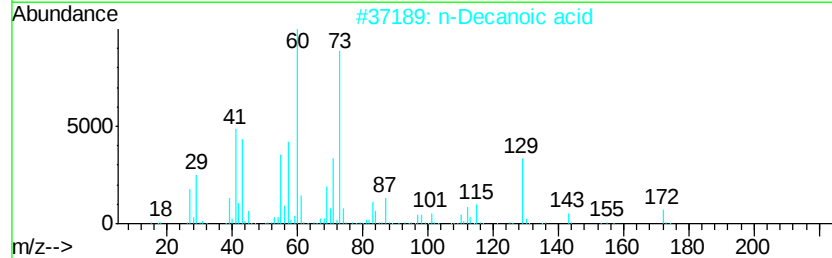
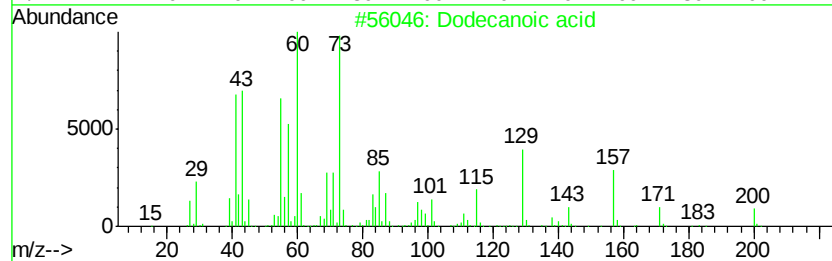
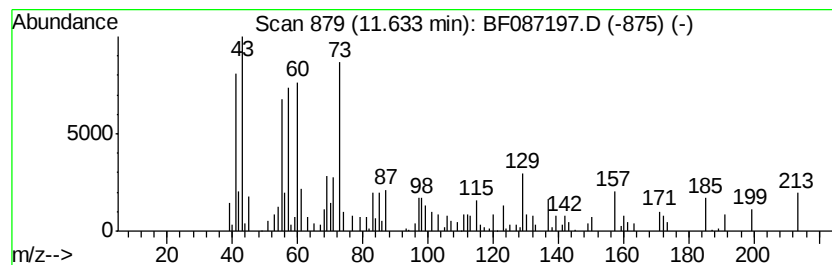
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dodecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	2.19 ng	133937	Phenanthrene-d10	11.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2		n-Decanoic acid	172	C10H20O2	000334-48-5	55
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43
4		Glucose	180	C6H12O6	000050-99-7	38
5		1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
Data File : BF087197.D
Acq On : 19 May 2016 20:06
Operator : UM/SJ
Sample : H3138-01
Misc :
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ClientSampleId :
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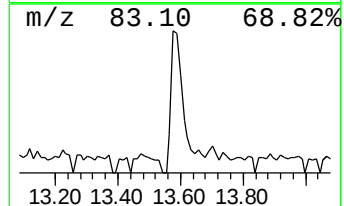
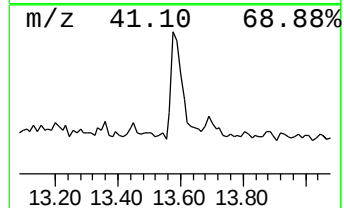
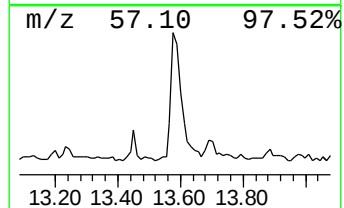
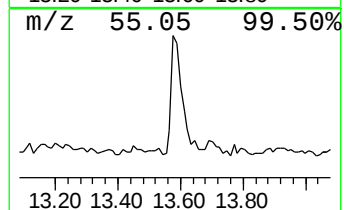
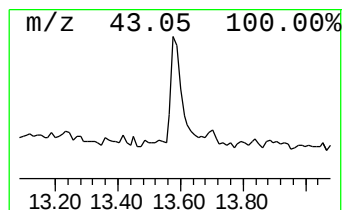
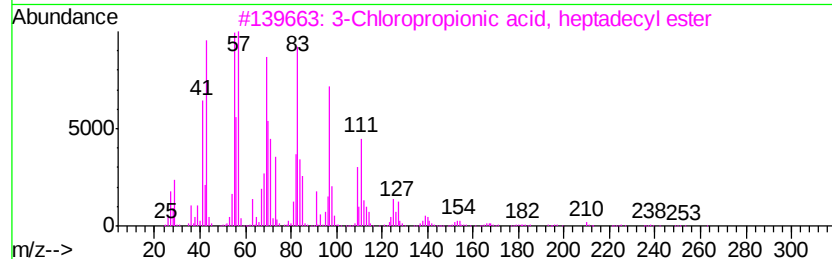
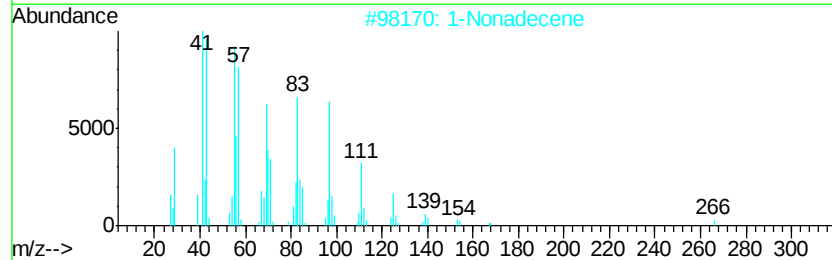
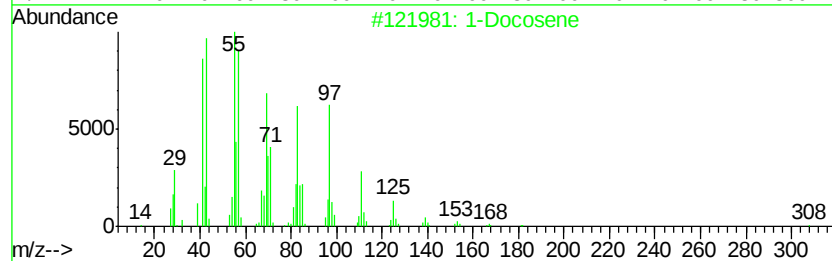
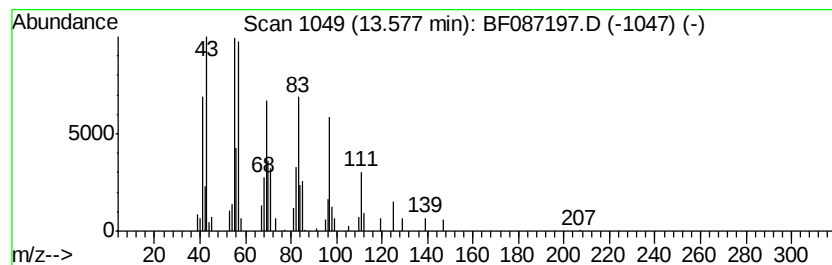
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	2.74 ng	125892	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4		Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	91
5		1-Heptadecanol	256	C17H36O	001454-85-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051916\
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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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unknown4.75	4.75	3.6	ng	227365	1	6.56	1249740	20.0
2-Octanol, 2-methyl-	6.30	4.3	ng	268100	1	6.56	1249740	20.0
unknown6.34	6.34	57.0	ng	3558660	1	6.56	1249740	20.0
2-Octanol, 2,6-di...	6.40	3.1	ng	192791	1	6.56	1249740	20.0
3-Heptanol, 3,5-d...	6.42	13.7	ng	857221	1	6.56	1249740	20.0
unknown6.64	6.64	7.6	ng	476777	1	6.56	1249740	20.0
7,9-Di-tert-butyl...	11.47	3.3	ng	203361	4	11.07	1222240	20.0
Dodecanoic acid	11.63	2.2	ng	133937	4	11.07	1222240	20.0
1-Docosene	13.58	2.7	ng	125892	5	13.70	917340	20.0