

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
 Data File : BF081250.D
 Acq On : 27 Aug 2015 17:04
 Operator : UM/IZ
 Sample : G3430-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB5(24-25)

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-BF081715.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	3.817	179	182	186	rBV	18880	32093	1.87%	0.210%
2	4.606	247	251	266	rVB	725989	1256911	73.43%	8.223%
3	5.074	289	292	294	rBV	1260280	1680393	98.17%	10.993%
4	5.497	327	329	331	rVB	27906	36594	2.14%	0.239%
5	6.160	384	387	389	rBV	1579069	1711744	100.00%	11.198%
6	6.275	394	397	399	rVV	1399531	1674743	97.84%	10.956%
7	6.355	403	404	410	rVB2	16465	18952	1.11%	0.124%
8	6.503	415	417	419	rBV	365903	295107	17.24%	1.931%
9	6.663	428	431	433	rBV	1057683	1110126	64.85%	7.262%
10	7.075	464	467	470	rBV	972445	947763	55.37%	6.200%
11	7.795	527	530	532	rVB	275857	373143	21.80%	2.441%
12	8.869	621	624	627	rBV	1547744	1436037	83.89%	9.395%
13	9.269	657	659	661	rBV	253104	198833	11.62%	1.301%
14	9.532	680	682	684	rBV	503136	436435	25.50%	2.855%
15	10.309	748	750	753	rBV2	772252	1079702	63.08%	7.063%
16	10.458	761	763	766	rVB	26161	28225	1.65%	0.185%
17	10.904	797	802	803	rBV	26665	24252	1.42%	0.159%
18	10.995	808	810	813	rBV	452374	431921	25.23%	2.826%
19	11.269	832	834	837	rBV	8523	18966	1.11%	0.124%
20	11.326	837	839	841	rVB	20827	18423	1.08%	0.121%
21	11.555	857	859	863	rBV	53579	75344	4.40%	0.493%
22	12.584	946	949	951	rBV	1608070	1506223	87.99%	9.854%
23	13.498	1026	1029	1036	rBV	96189	173631	10.14%	1.136%
24	13.612	1036	1039	1041	rBV	333676	408964	23.89%	2.675%
25	14.470	1112	1114	1116	rVB	28932	25099	1.47%	0.164%
26	14.938	1152	1155	1157	rBV	193408	286138	16.72%	1.872%

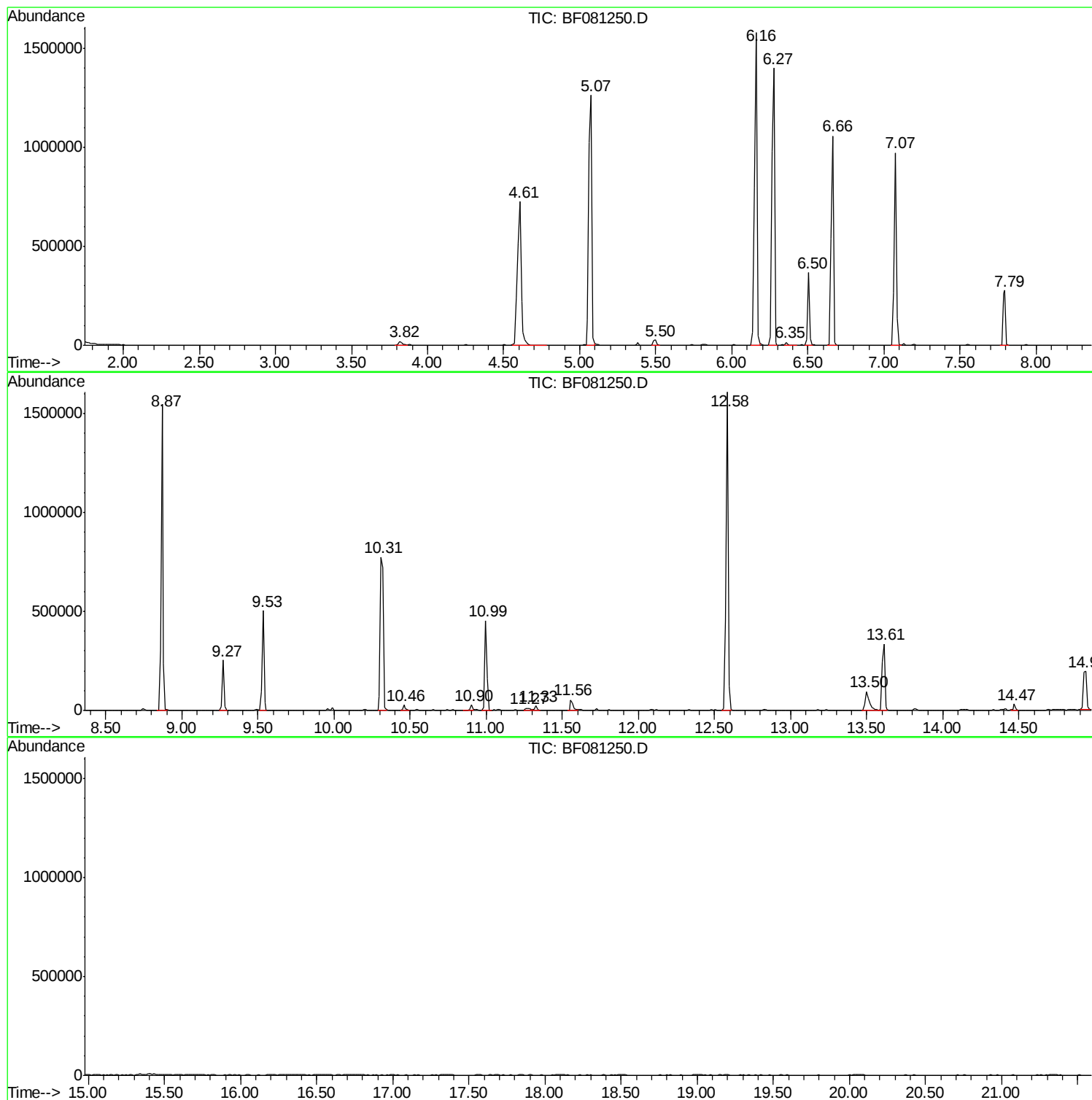
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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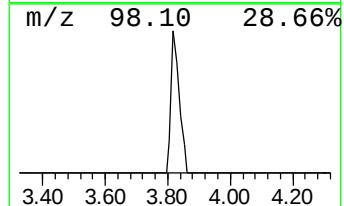
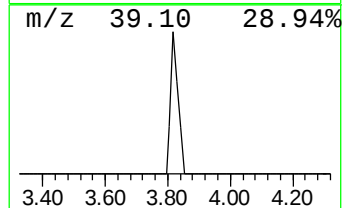
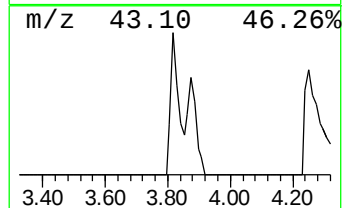
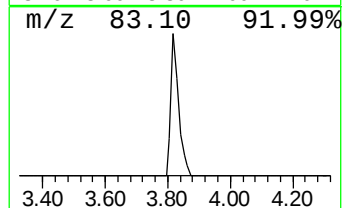
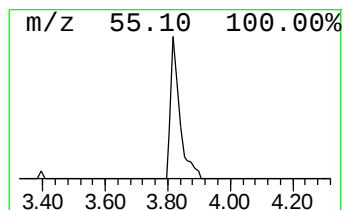
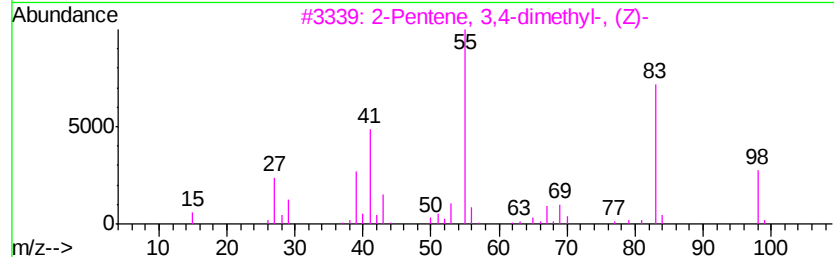
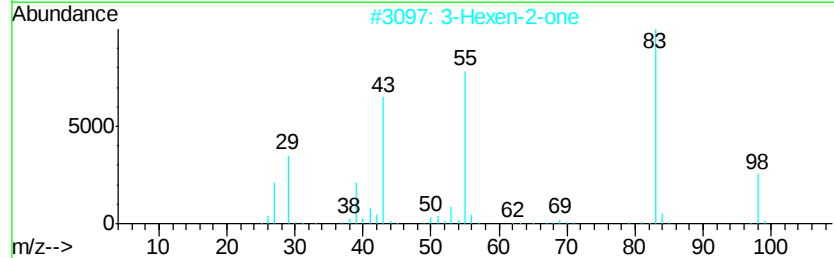
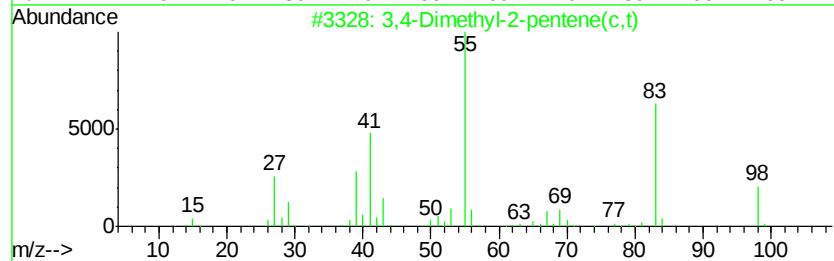
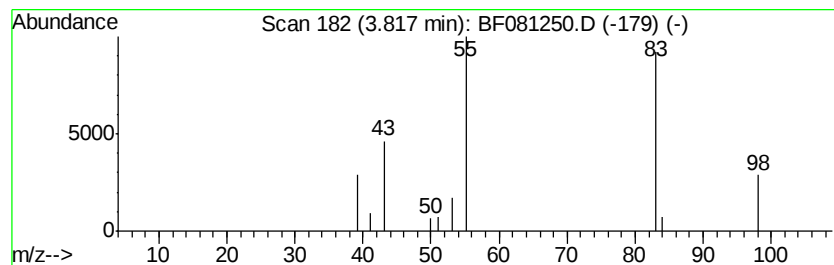
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3,4-Dimethyl-2-pentene(c,t) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.82	2.18 ng	32093	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	90
5		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90



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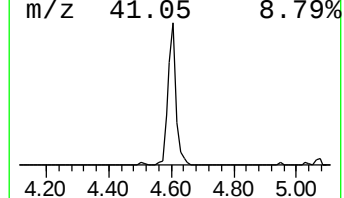
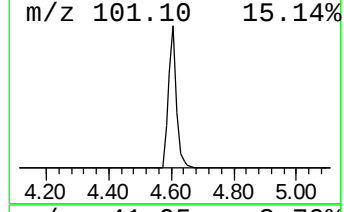
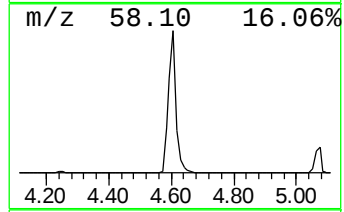
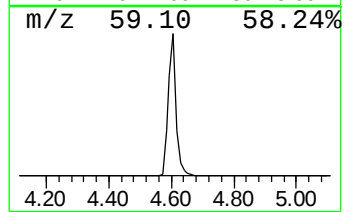
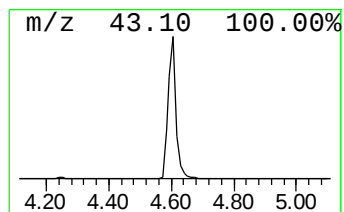
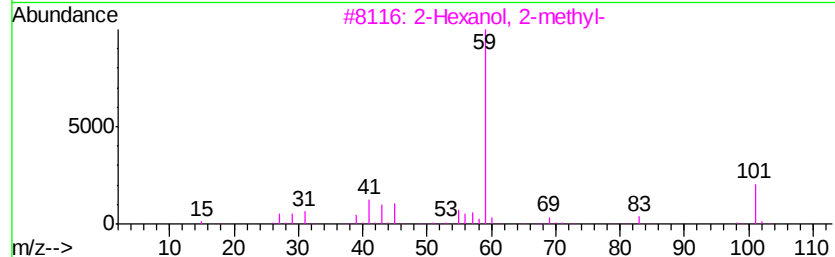
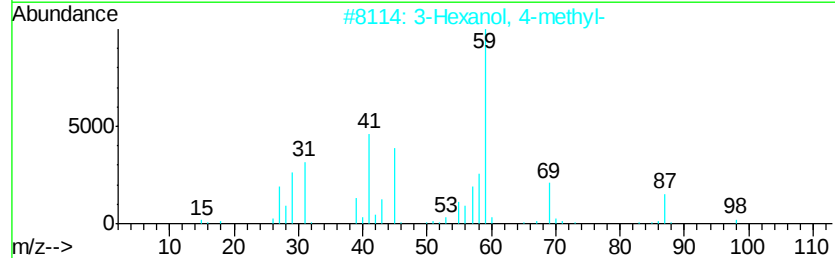
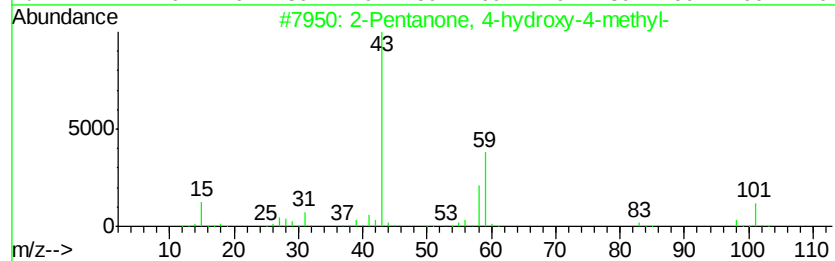
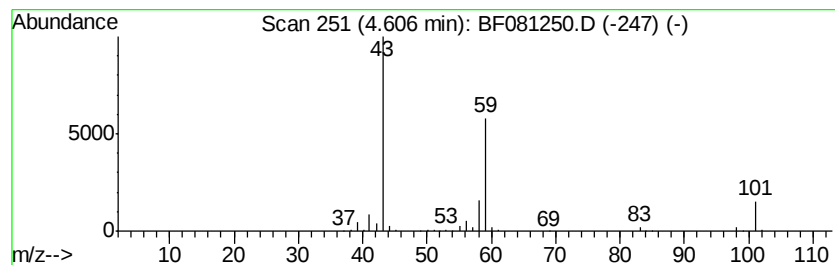
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	85.18 ng	1256910	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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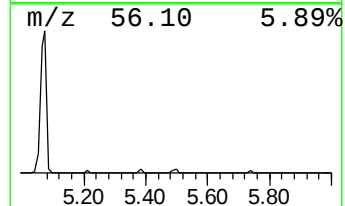
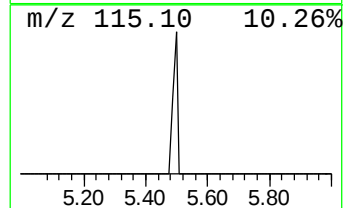
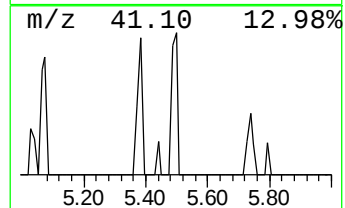
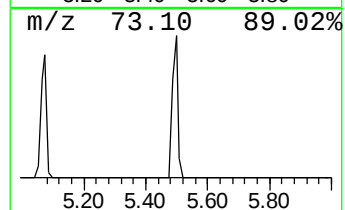
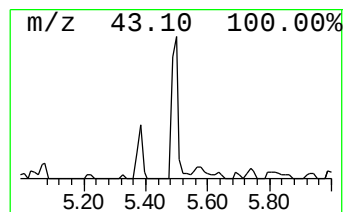
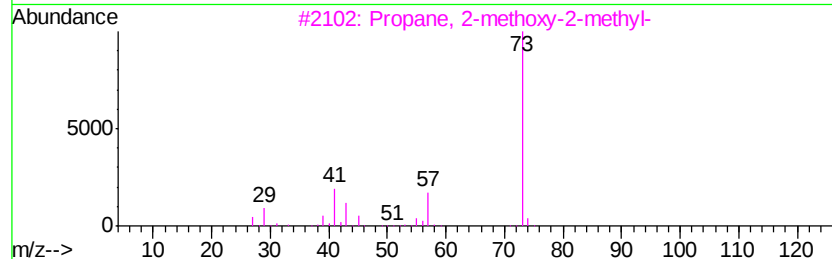
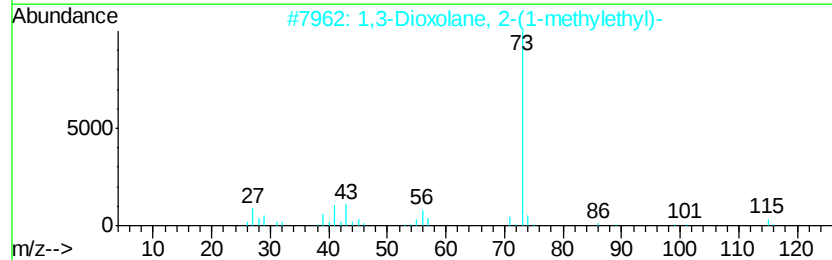
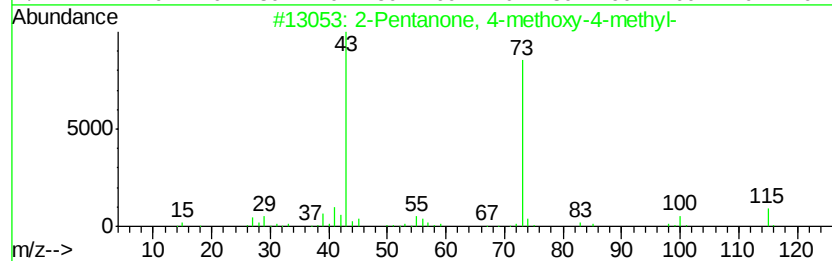
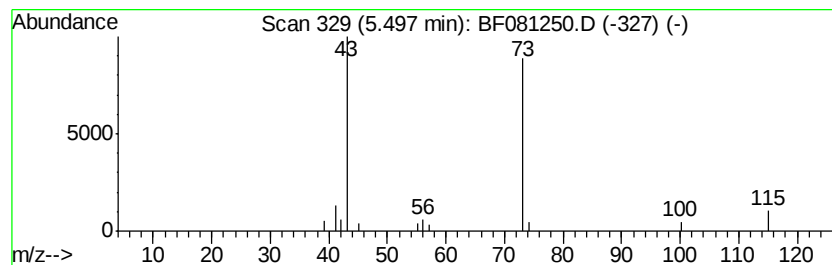
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.50	2.48 ng	36594	1,4-Dichlorobenzene-d4	6.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Guanidine, methyl-	73	C2H7N3	000471-29-4	7
5		N-Ethylformamide	73	C3H7NO	000627-45-2	7



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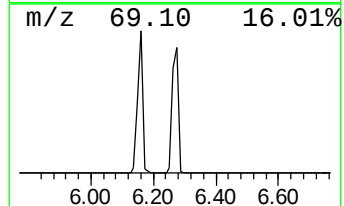
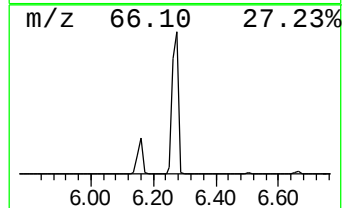
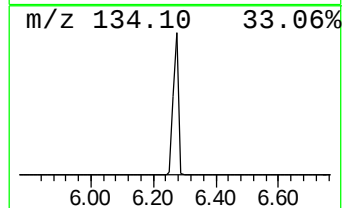
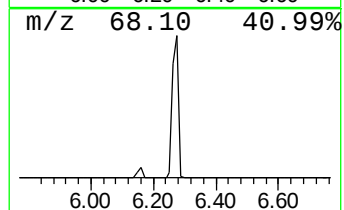
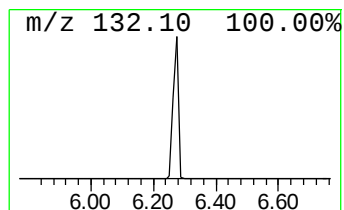
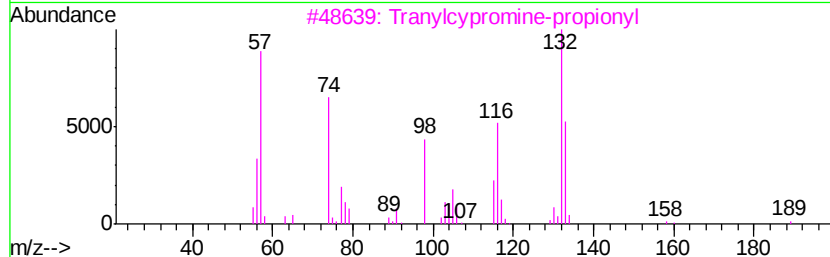
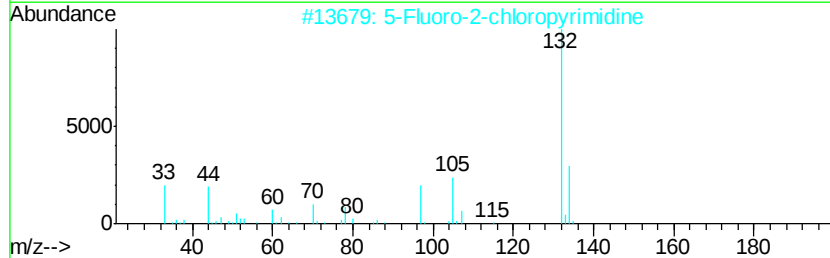
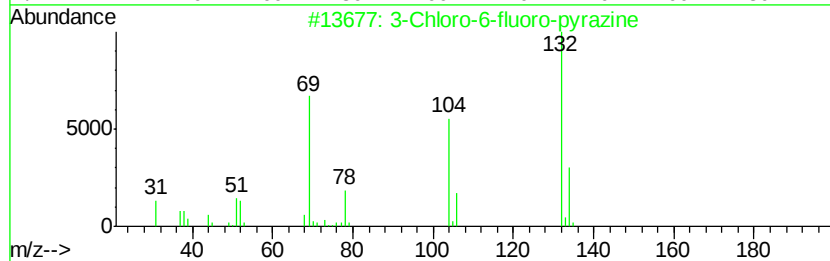
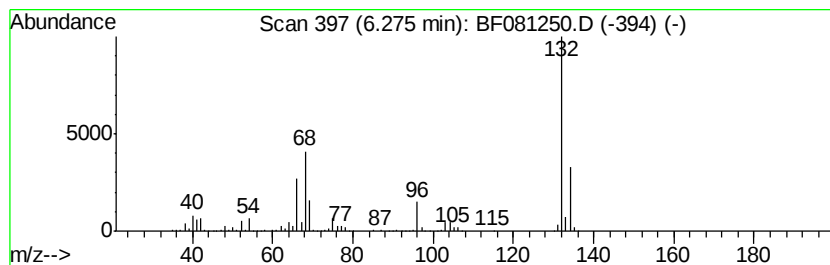
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	113.50 ng	1674740	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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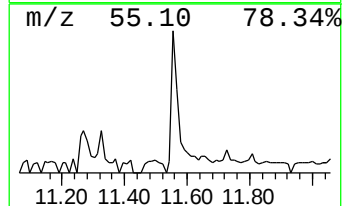
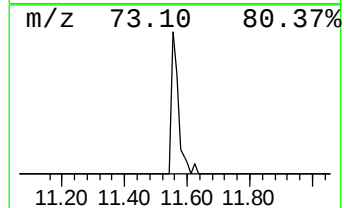
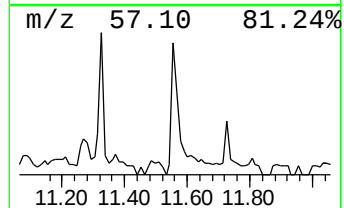
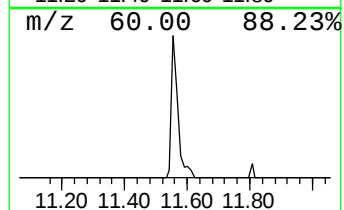
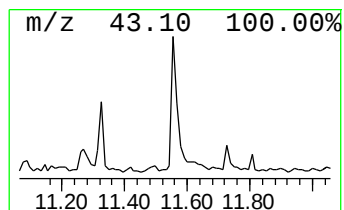
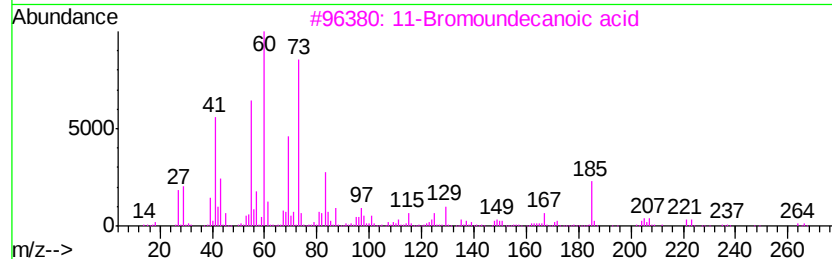
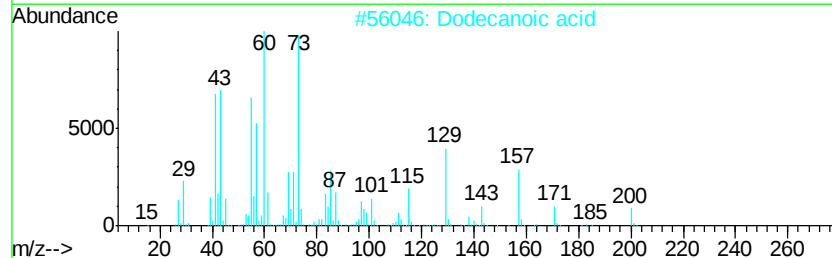
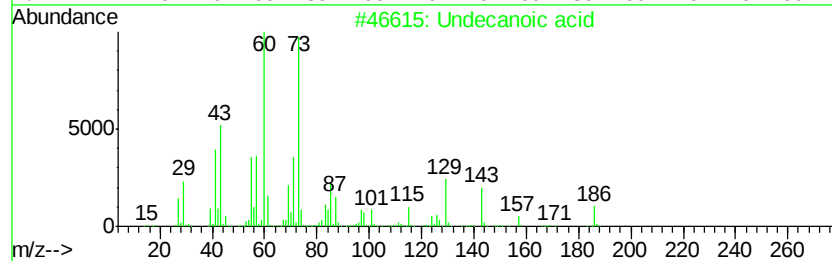
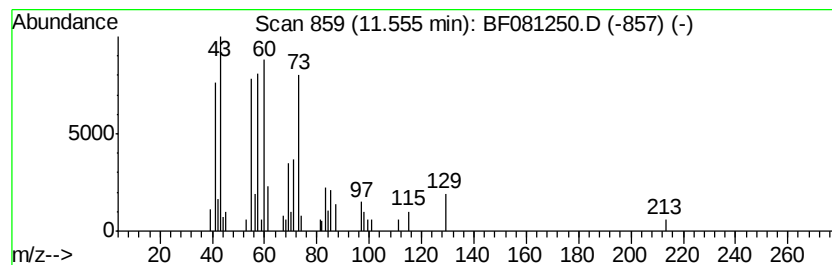
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	3.49 ng	75344	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecanoic acid	186	C11H22O2	000112-37-8	72
2		Dodecanoic acid	200	C12H24O2	000143-07-7	64
3		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	53
4		n-Decanoic acid	172	C10H20O2	000334-48-5	50
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	43



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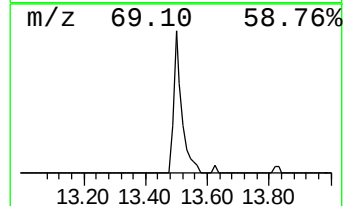
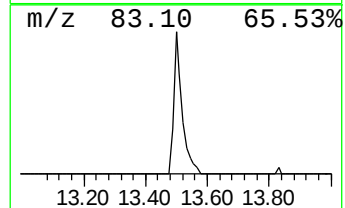
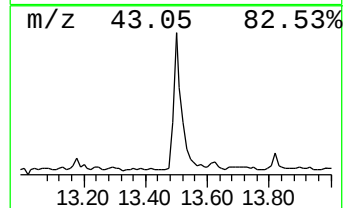
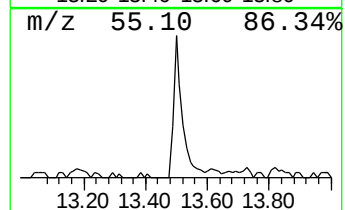
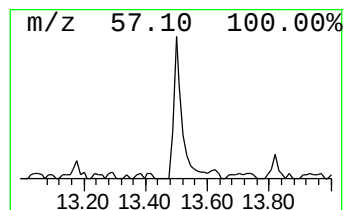
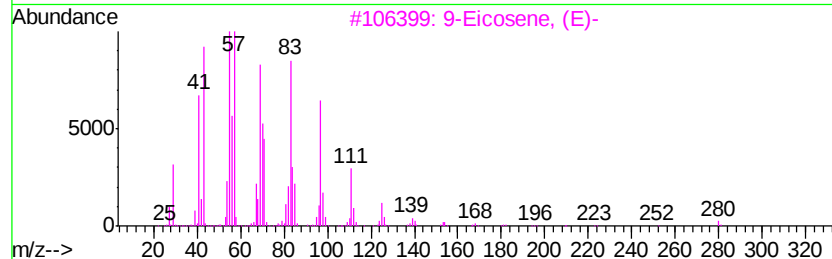
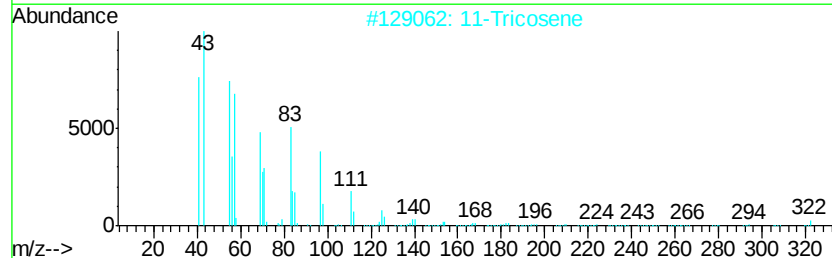
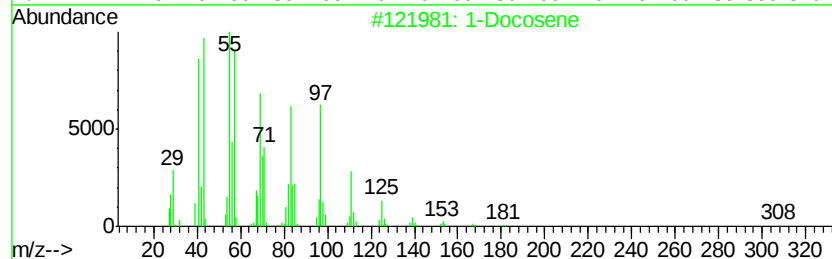
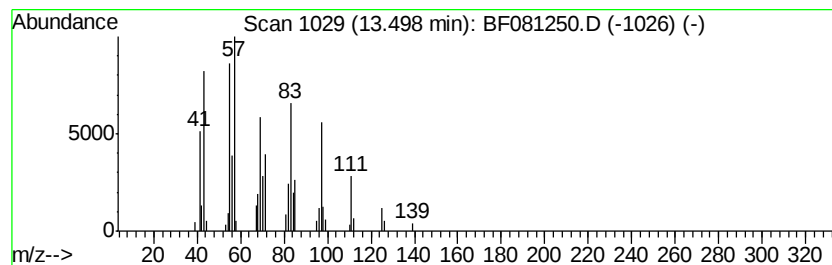
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	8.49 ng	173631	Chrysene-d12	13.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	90
2	11-Tricosene		322	C23H46	052078-56-5	87
3	9-Eicosene, (E)-		280	C20H40	074685-29-3	86
4	1-Tetracosanol		354	C24H50O	000506-51-4	80
5	1-Hexacosanol		382	C26H54O	000506-52-5	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
Data File : BF081250.D
Acq On : 27 Aug 2015 17:04
Operator : UM/IZ
Sample : G3430-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB5(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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
3,4-Dimethyl-2-pe...	3.82	2.2	ng	32093	1	6.50	295107	20.0
2-Pentanone, 4-hy...	4.61	85.2	ng	1256910	1	6.50	295107	20.0
2-Pentanone, 4-me...	5.50	2.5	ng	36594	1	6.50	295107	20.0
unknown6.27	6.27	113.5	ng	1674740	1	6.50	295107	20.0
Undecanoic acid	11.56	3.5	ng	75344	4	10.99	431921	20.0
1-Docosene	13.50	8.5	ng	173631	5	13.61	408964	20.0