

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042016\
 Data File : BF086316.D
 Acq On : 20 Apr 2016 18:45
 Operator : UM/SJ
 Sample : H2625-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-8

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-BF042016.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	5.036	256	258	265	rBV	628122	785997	10.88%	1.630%
2	5.447	292	294	297	rBV	2216370	2848978	39.45%	5.909%
3	5.859	329	330	333	rBV	190874	204650	2.83%	0.424%
4	5.950	335	338	345	rVB	25891	72872	1.01%	0.151%
5	6.487	382	385	394	rBV	1319080	2133277	29.54%	4.424%
6	6.624	394	397	400	rBV	4613259	4997713	69.20%	10.365%
7	6.864	415	418	429	rVB	1039057	1568456	21.72%	3.253%
8	7.013	429	431	434	rBV	3799597	4634446	64.17%	9.612%
9	7.425	464	467	483	rBV	3482506	4526641	62.68%	9.388%
10	8.145	528	530	539	rBV	1945056	2098157	29.05%	4.351%
11	9.230	622	625	627	rBV	5494640	7221888	100.00%	14.978%
12	9.619	654	659	664	rVB2	58671	95115	1.32%	0.197%
13	9.905	681	684	686	rBV	1397623	2041268	28.27%	4.233%
14	10.339	718	722	724	rBV2	119691	163968	2.27%	0.340%
15	10.682	750	752	755	rBV2	2502405	3850661	53.32%	7.986%
16	10.808	761	763	770	rVB	151844	208839	2.89%	0.433%
17	11.254	800	802	808	rBV3	49852	105894	1.47%	0.220%
18	11.379	811	813	817	rBV	1706797	1859514	25.75%	3.856%
19	11.562	826	829	837	rVB	110938	179736	2.49%	0.373%
20	11.688	837	840	851	rVB4	26175	110563	1.53%	0.229%
21	12.625	919	922	927	rBV	245579	256340	3.55%	0.532%
22	12.968	949	952	960	rBV	4479816	5265328	72.91%	10.920%
23	13.539	997	1002	1003	rBV2	51682	74525	1.03%	0.155%
24	13.574	1003	1005	1007	rVB	101504	114387	1.58%	0.237%
25	13.951	1034	1038	1041	rBV	60831	163200	2.26%	0.338%
26	14.008	1041	1043	1051	rVB	1000434	1383666	19.16%	2.870%
27	15.437	1165	1168	1177	rBV	851808	1251624	17.33%	2.596%

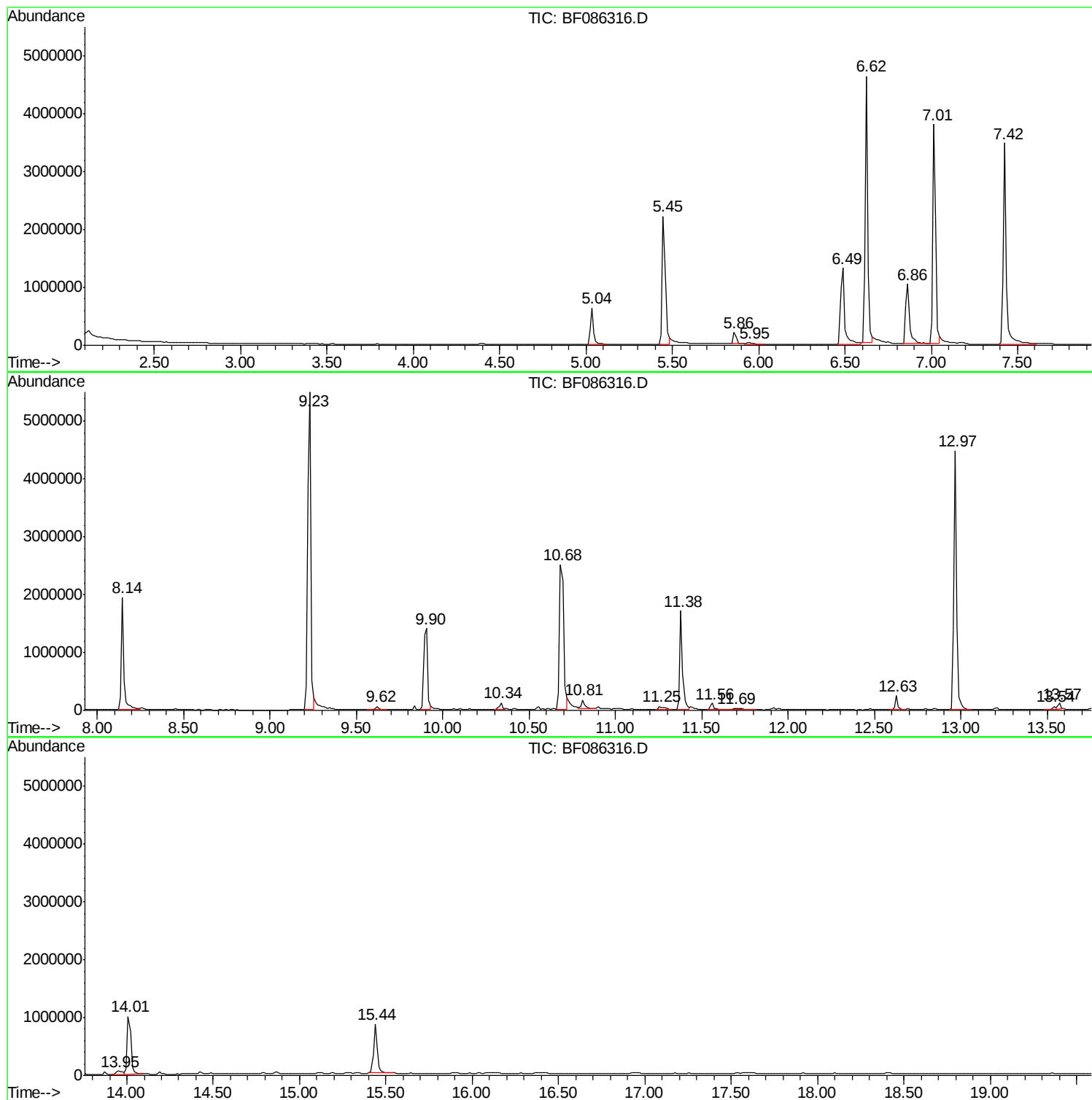
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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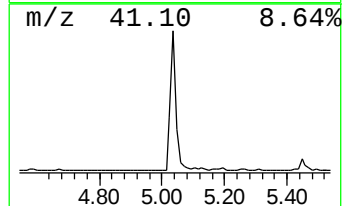
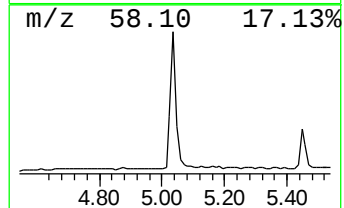
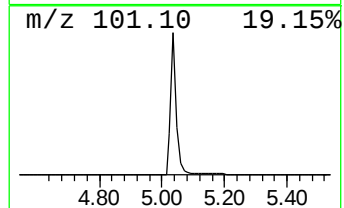
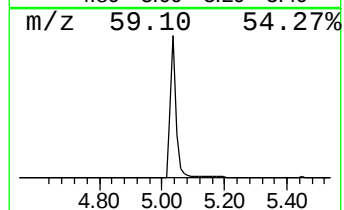
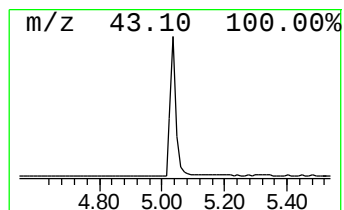
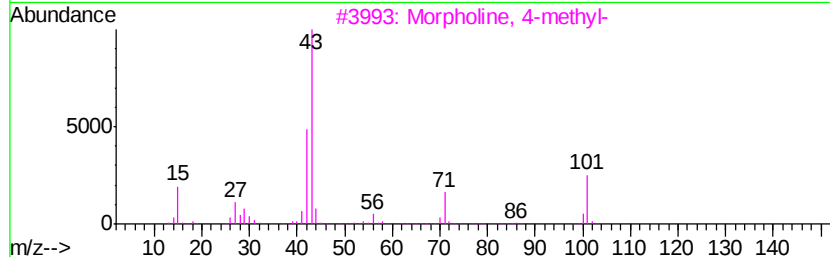
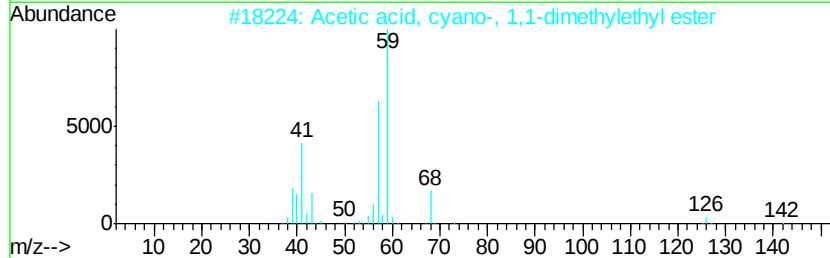
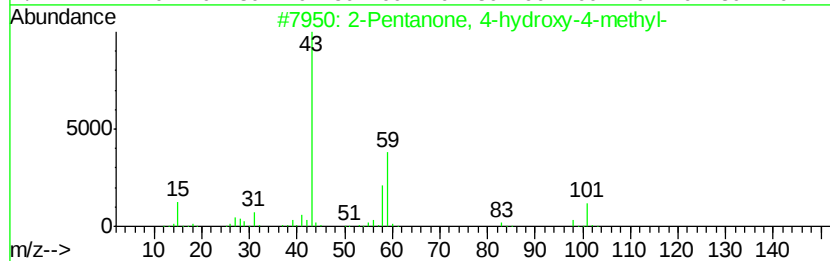
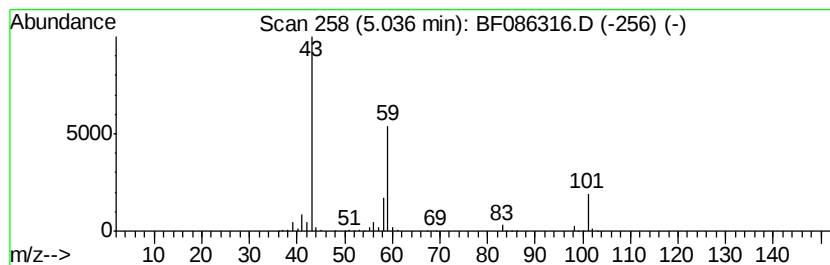
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	10.02 ng	785997	1,4-Dichlorobenzene-d4	6.86

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		1,2-Butanediol, (./-.)-	90	C4H10O2	026171-83-5	9
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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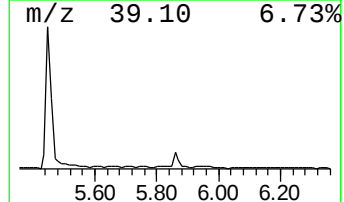
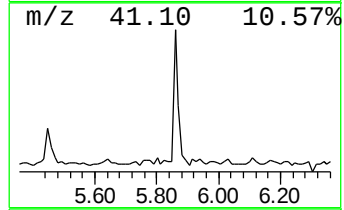
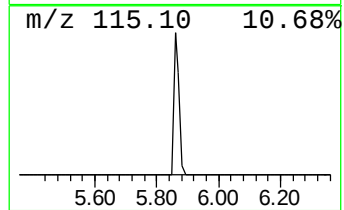
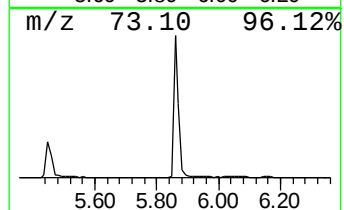
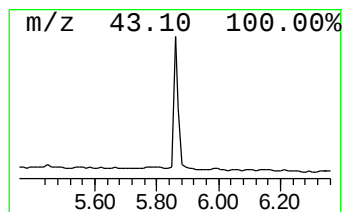
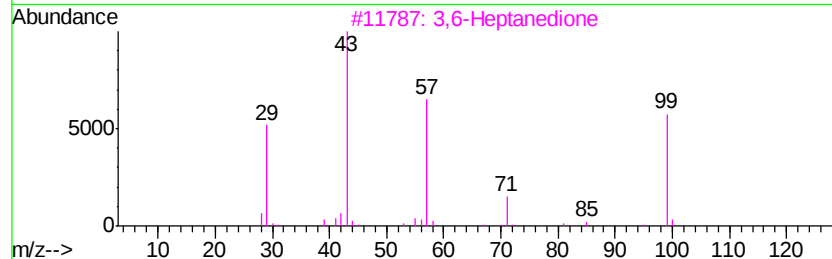
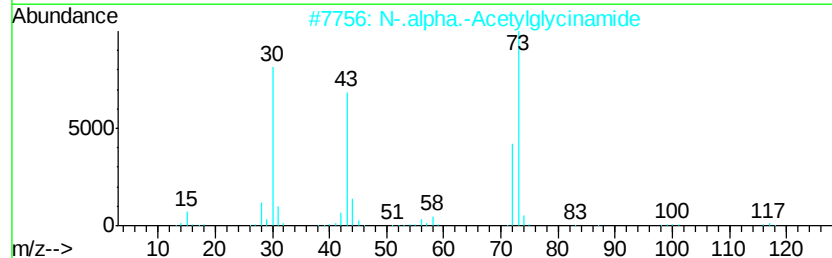
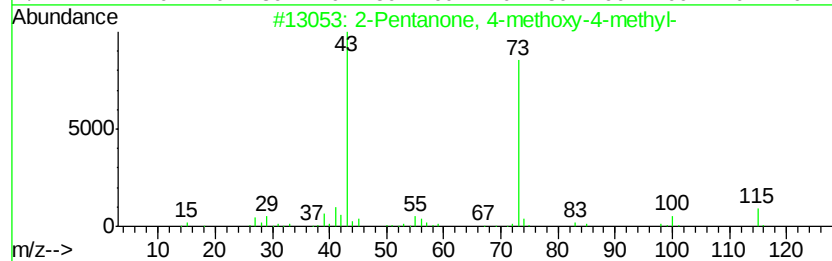
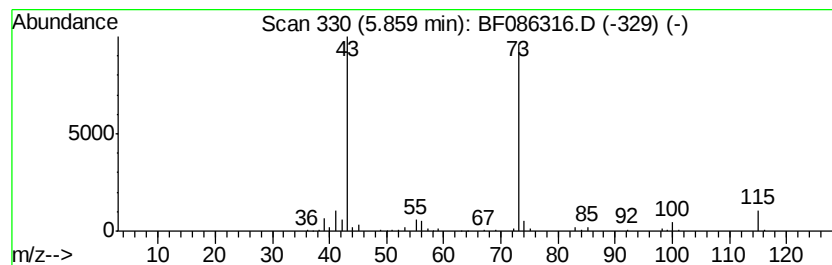
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.61 ng	204650	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglucynamide	116	C4H8N2O2	002620-63-5	38
3		3,6-Heptanedione	128	C7H12O2	001703-51-1	17
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	16
5		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10



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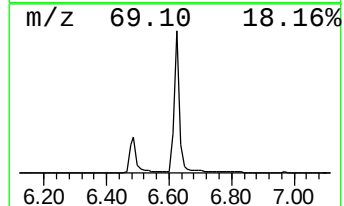
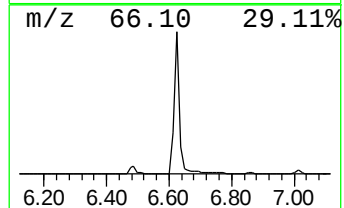
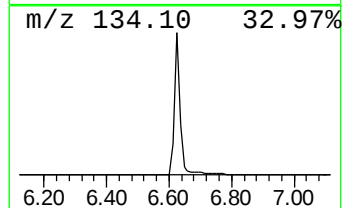
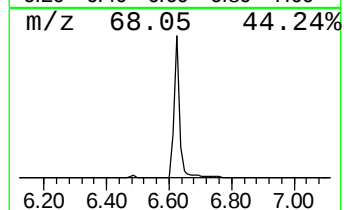
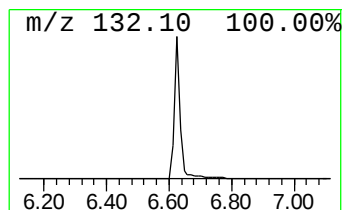
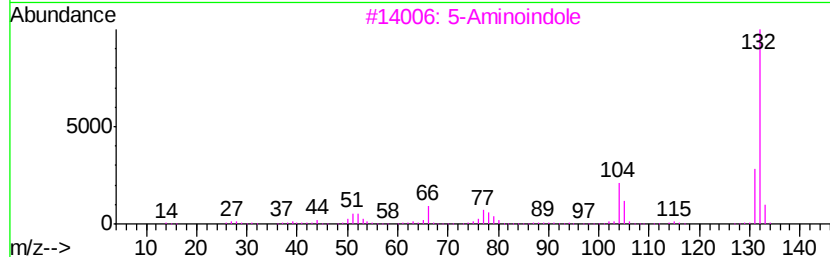
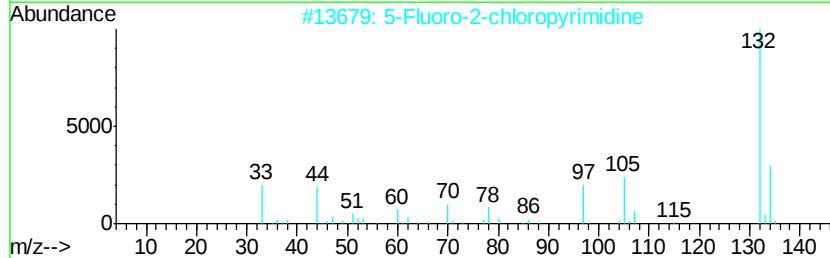
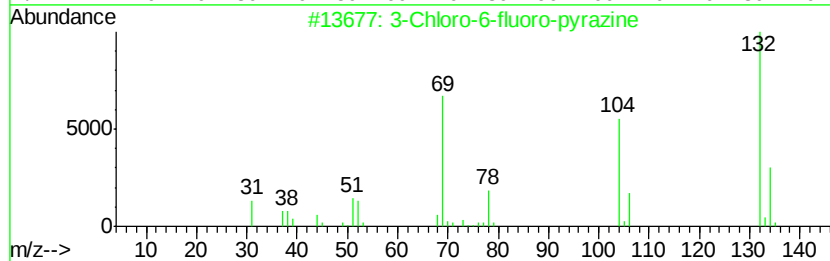
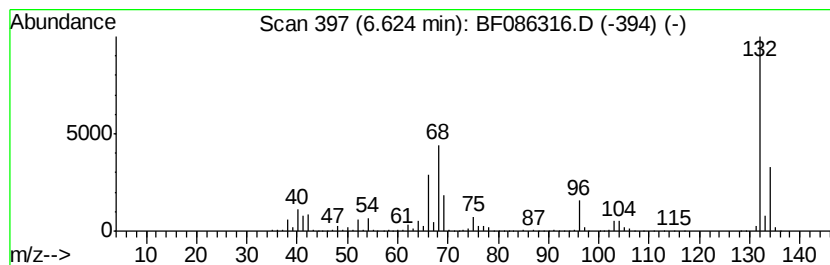
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Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	63.73 ng	4997710	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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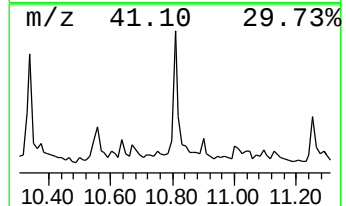
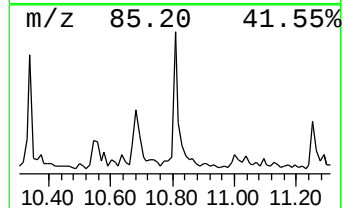
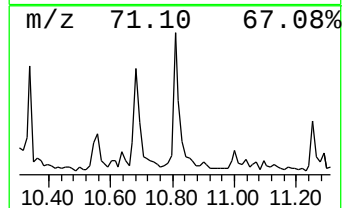
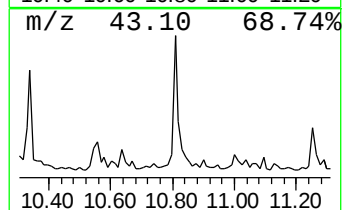
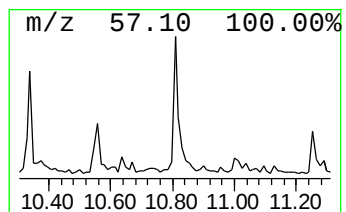
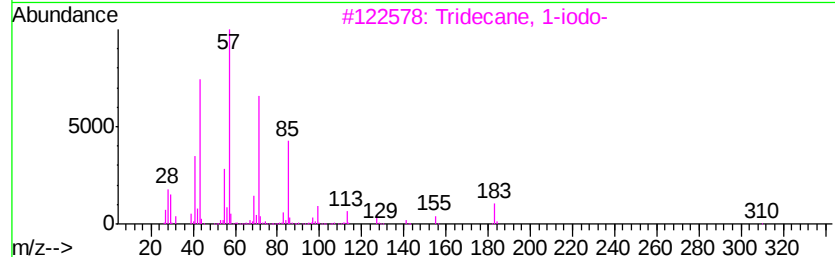
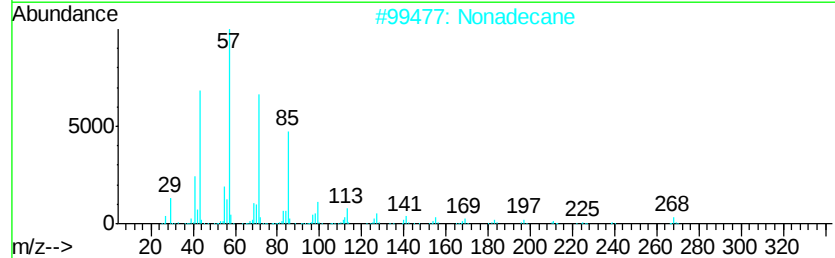
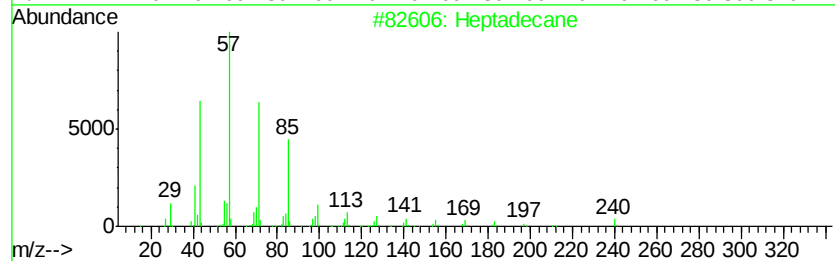
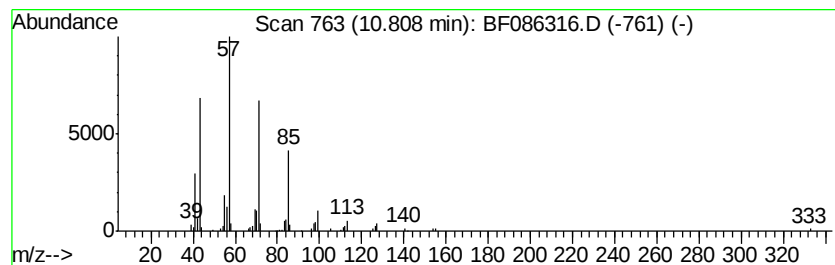
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.25 ng	208839	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Nonadecane		268	C19H40	000629-92-5	90
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90
4	Octacosane		394	C28H58	000630-02-4	86
5	Eicosane		282	C20H42	000112-95-8	86



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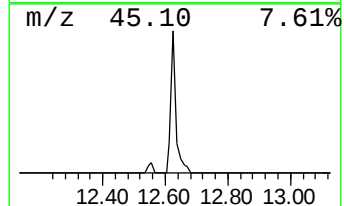
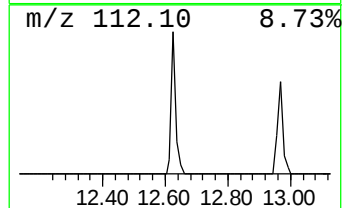
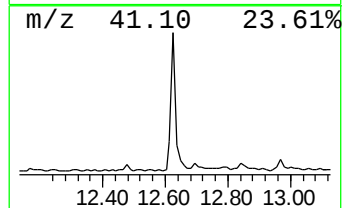
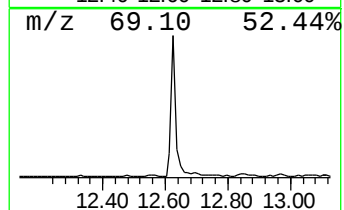
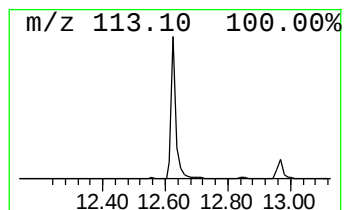
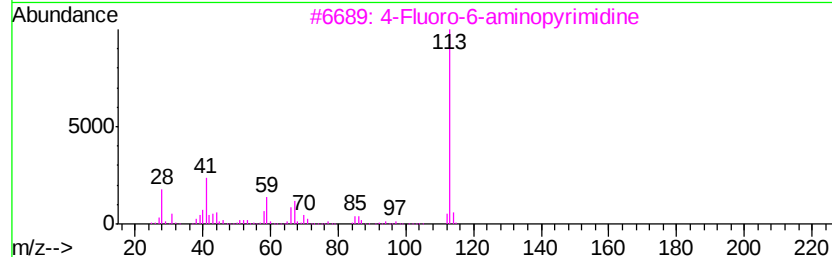
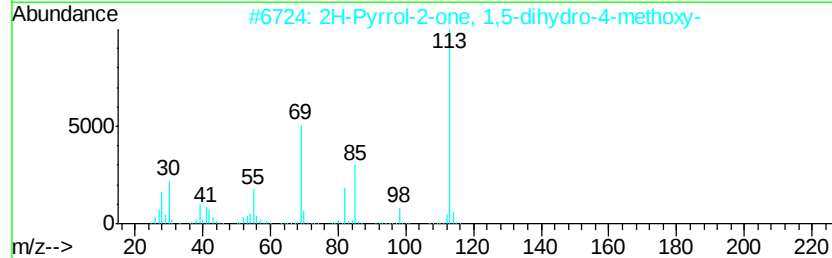
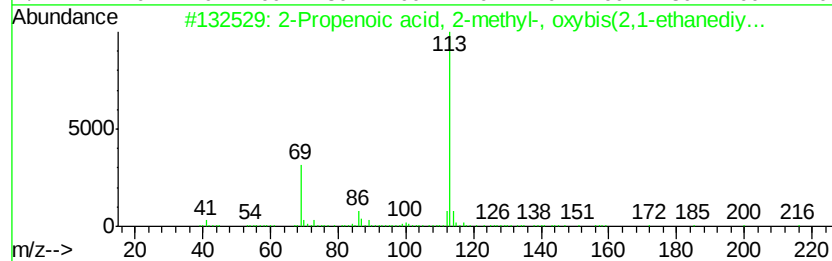
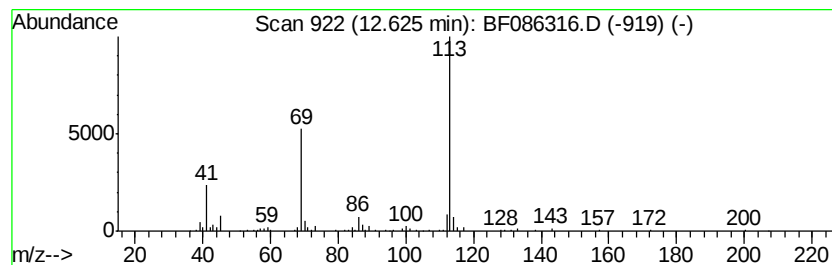
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Propenoic acid, 2-methyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	2.76 ng	256340	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenoic acid, 2-methyl-, oxv...	330	C16H26O7	000109-17-1	86
2		2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	72
3		4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	64
4		Thiazole, 4,5-dimethyl-	113	C5H7NS	003581-91-7	50
5		3-Methoxy-1H-pyrazol-5-ylacetamide	155	C6H9N3O2	1000284-55-3	50



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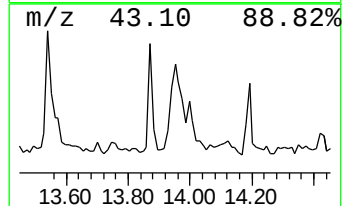
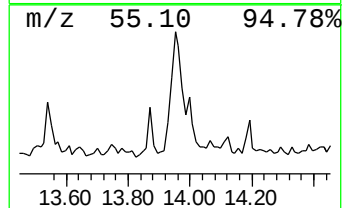
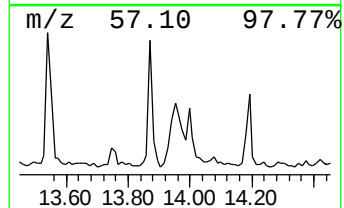
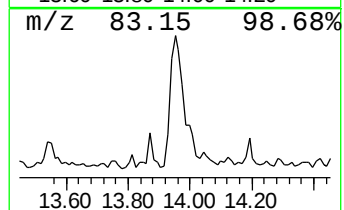
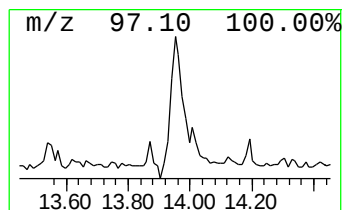
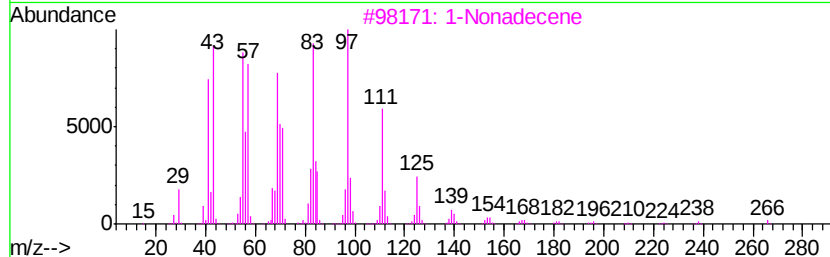
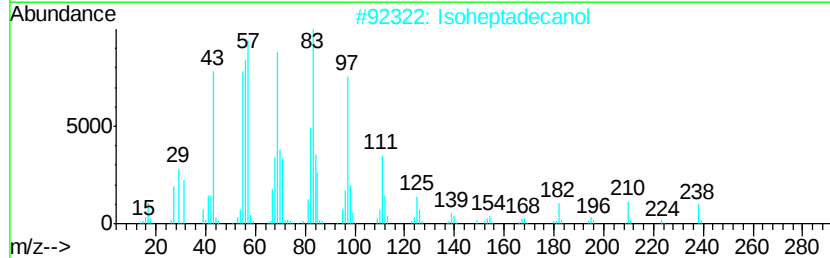
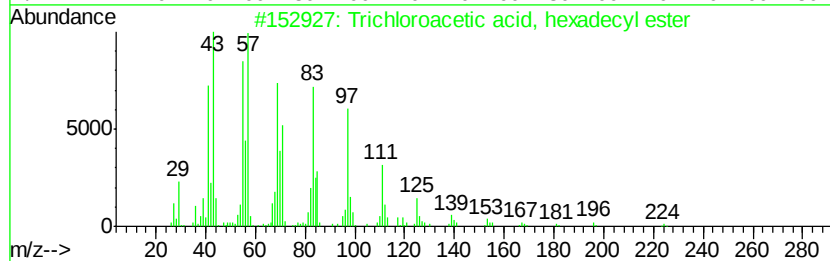
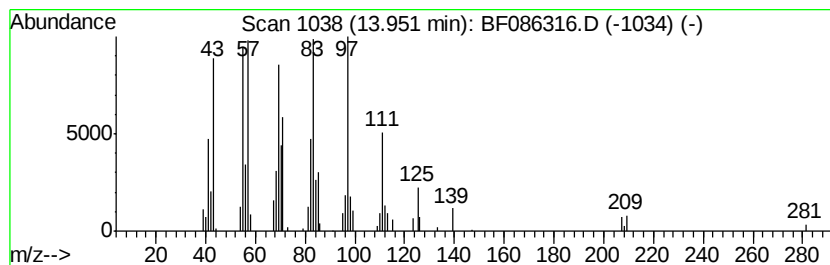
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.36 ng	163200	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
2		Isoheptadecanol	256	C17H36O	057289-07-3	83
3		1-Nonadecene	266	C19H38	018435-45-5	76
4		1-Docosene	308	C22H44	001599-67-3	76
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042016\
Data File : BF086316.D
Acq On : 20 Apr 2016 18:45
Operator : UM/SJ
Sample : H2625-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	10.0	ng	785997	1	6.86	1568460	20.0
2-Pentanone, 4-me...	5.86	2.6	ng	204650	1	6.86	1568460	20.0
unknown6.62	6.62	63.7	ng	4997710	1	6.86	1568460	20.0
Heptadecane	10.81	2.3	ng	208839	4	11.38	1859510	20.0
2-Propenoic acid,...	12.63	2.8	ng	256340	4	11.38	1859510	20.0
Trichloroacetic a...	13.95	2.4	ng	163200	5	14.01	1383670	20.0