

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
 Data File : BF086258.D
 Acq On : 16 Apr 2016 11:39
 Operator : UM/SJ
 Sample : H2471-02
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CDMSH2

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-BF041516.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	2.167	5	7	24	rVB	283103	535768	8.18%	0.902%
2	5.093	261	263	270	rVB	266529	400732	6.12%	0.675%
3	5.493	295	298	300	rBV	5577423	6274476	95.81%	10.563%
4	6.522	384	388	390	rBV	5443178	6549201	100.00%	11.025%
5	6.659	397	400	402	rBV	5862568	5914194	90.30%	9.956%
6	6.887	418	420	423	rVB	1554561	1677897	25.62%	2.825%
7	7.047	431	434	437	rBV	4712984	4389844	67.03%	7.390%
8	7.459	467	470	472	rBV	3903659	4518888	69.00%	7.607%
9	7.493	472	473	475	rVV	79614	87963	1.34%	0.148%
10	7.539	475	477	479	rVB	100096	105182	1.61%	0.177%
11	8.179	530	533	535	rBV	2658386	2361792	36.06%	3.976%
12	9.253	624	627	630	rBV	5072844	5348773	81.67%	9.004%
13	9.653	659	662	664	rBV	700302	937249	14.31%	1.578%
14	9.870	679	681	683	rBV	224011	176522	2.70%	0.297%
15	9.928	684	686	689	rVB	2292383	2564176	39.15%	4.317%
16	10.099	699	701	703	rBV2	44086	72602	1.11%	0.122%
17	10.373	721	725	726	rBV	223802	314685	4.80%	0.530%
18	10.591	741	744	747	rBV	110560	189478	2.89%	0.319%
19	10.716	752	755	758	rBV	3340861	3423215	52.27%	5.763%
20	10.842	764	766	771	rVB	355044	392648	6.00%	0.661%
21	11.288	803	805	806	rBV	214649	167567	2.56%	0.282%
22	11.413	814	816	818	rBV	2739708	2403172	36.69%	4.046%
23	11.939	861	862	865	rBV	142351	235252	3.59%	0.396%
24	12.625	919	922	923	rBV	79710	111443	1.70%	0.188%
25	12.831	937	940	943	rBV2	221661	405190	6.19%	0.682%
26	13.002	952	955	957	rBV	4371644	4640633	70.86%	7.812%
27	13.242	972	976	977	rBV3	42429	70057	1.07%	0.118%
28	13.528	999	1001	1004	rBV2	124429	177534	2.71%	0.299%
29	13.574	1004	1005	1010	rVB	41041	71882	1.10%	0.121%
30	13.905	1031	1034	1042	rBV	375743	578553	8.83%	0.974%
31	14.042	1044	1046	1052	rVB	1660100	1666591	25.45%	2.806%
32	14.225	1059	1062	1064	rBV	69933	74775	1.14%	0.126%
33	14.534	1087	1089	1094	rBV	106438	181020	2.76%	0.305%
34	14.900	1119	1121	1125	rBV	62833	82595	1.26%	0.139%

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Stop Thrs : 0 Peak Location: TOP

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35	14.968	1125	1127	1130	rBV	122961	143834	2.20%	0.242%
36	15.060	1133	1135	1141	rVB	29092	67151	1.03%	0.113%
37	15.185	1141	1146	1154	rBV2	128624	315398	4.82%	0.531%
38	15.482	1169	1172	1175	rBV	1033232	1355117	20.69%	2.281%
39	15.963	1210	1214	1216	rBV	77465	150040	2.29%	0.253%
40	16.008	1216	1218	1222	rVB2	52424	105223	1.61%	0.177%
41	17.483	1343	1347	1353	rBV7	35674	89212	1.36%	0.150%
42	19.483	1518	1522	1527	rVB7	26101	74456	1.14%	0.125%

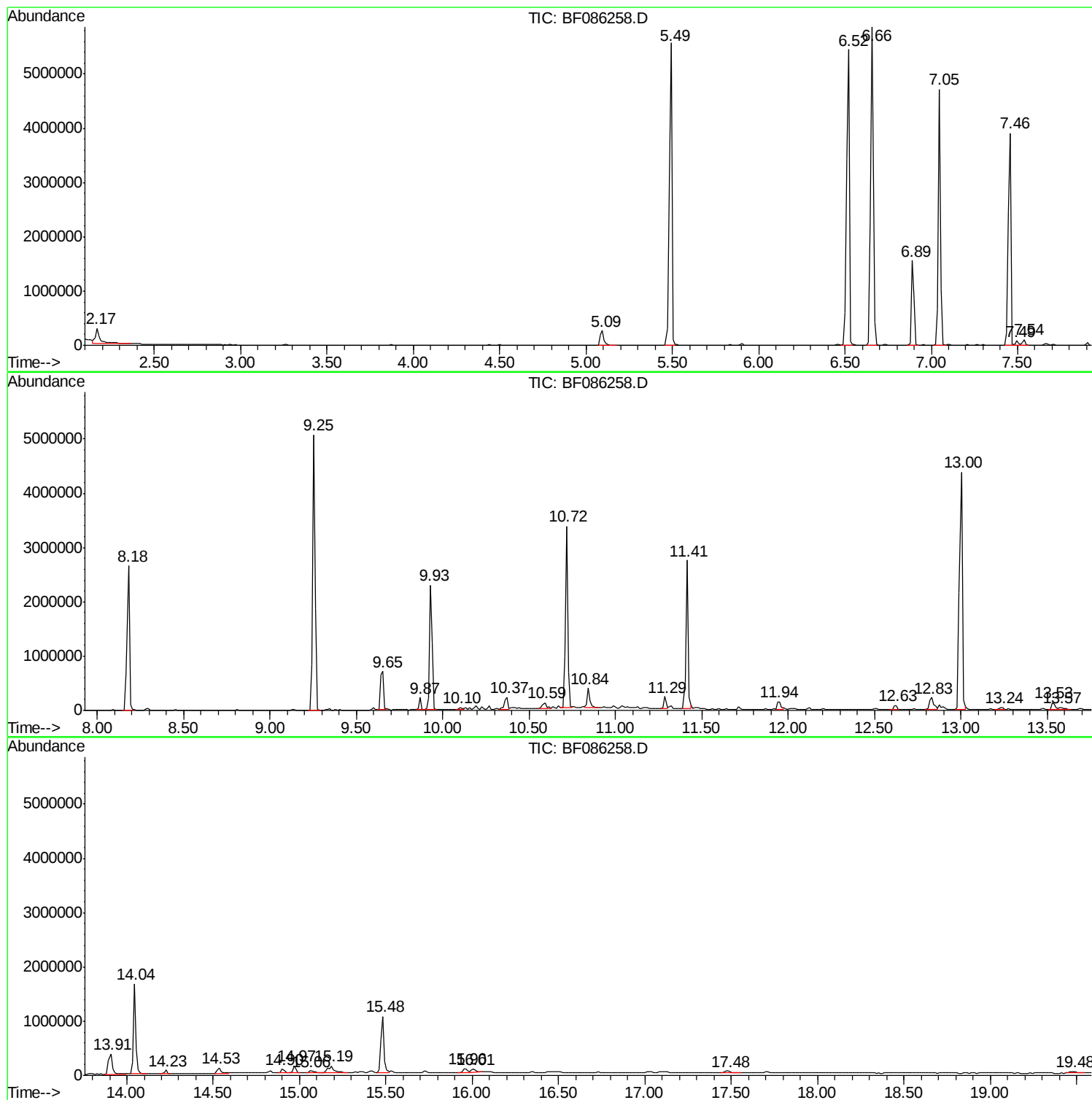
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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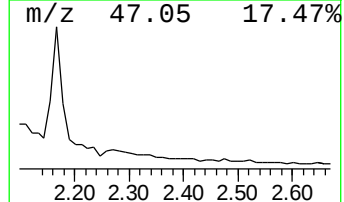
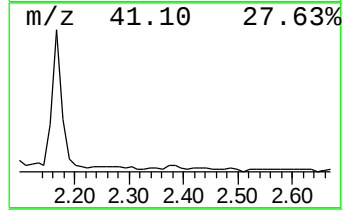
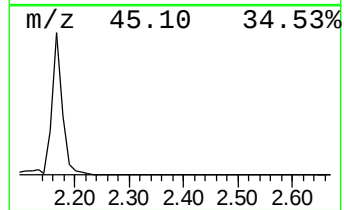
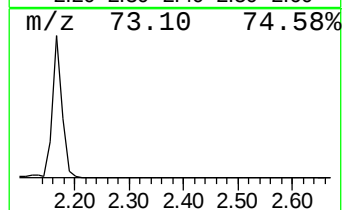
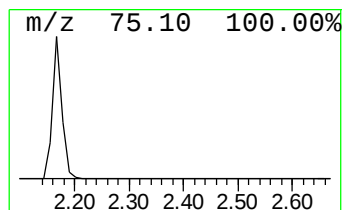
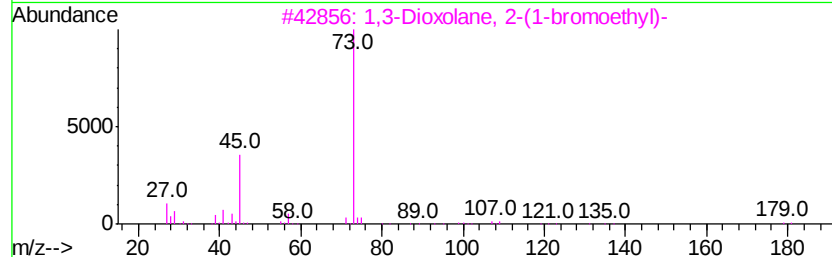
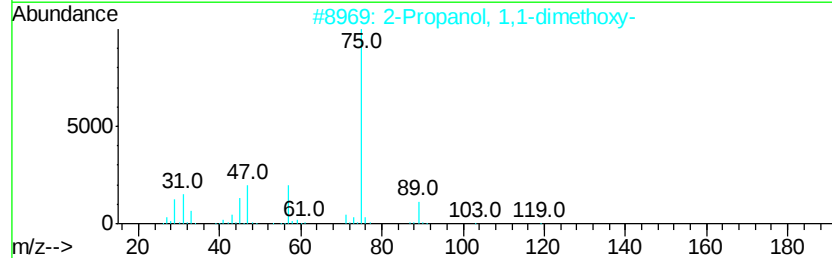
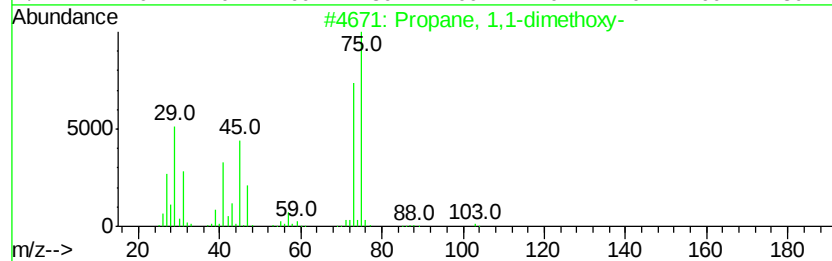
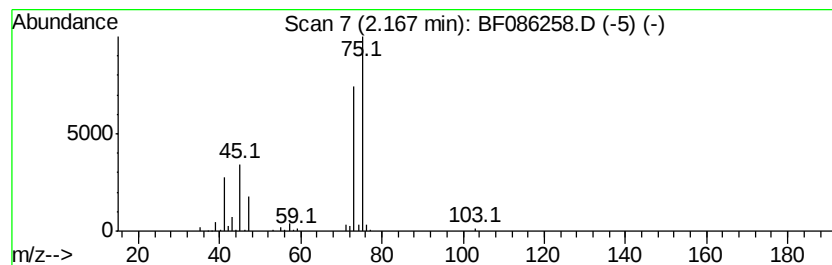
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	6.39 ng	535768	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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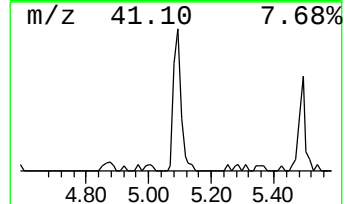
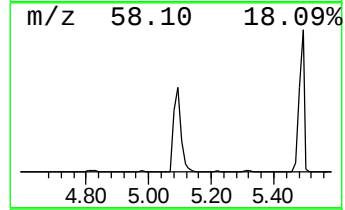
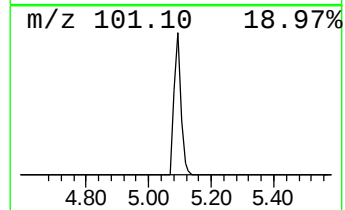
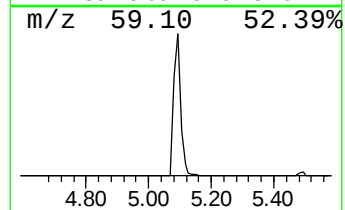
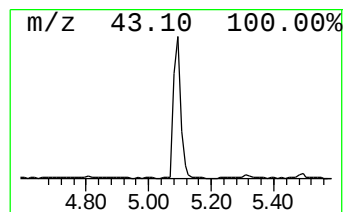
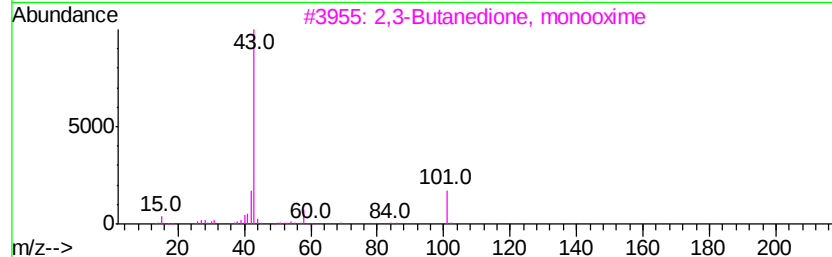
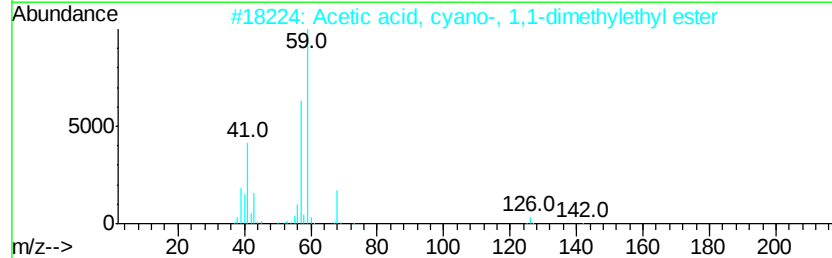
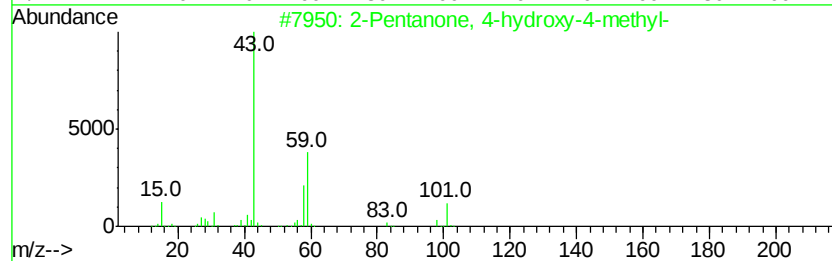
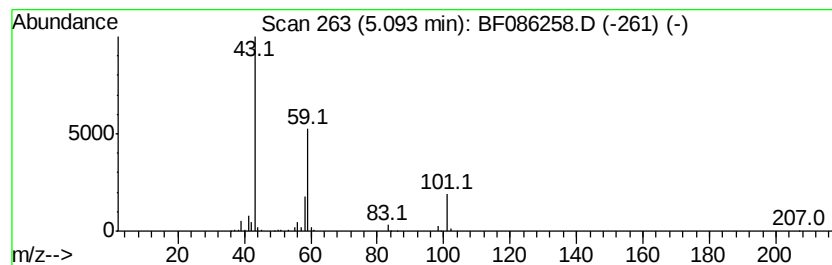
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.78 ng	400732	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		Acetone	58	C3H6O	000067-64-1	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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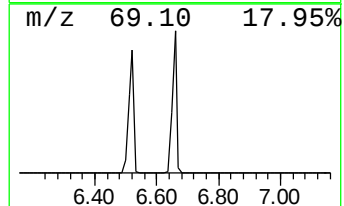
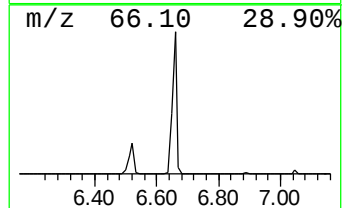
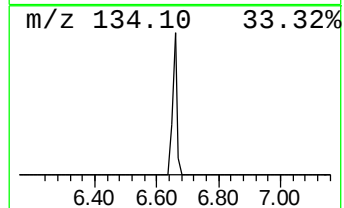
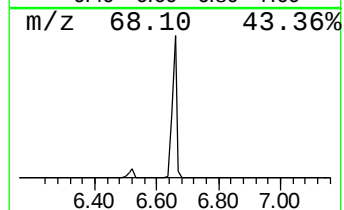
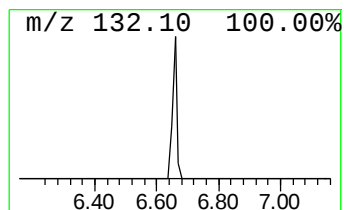
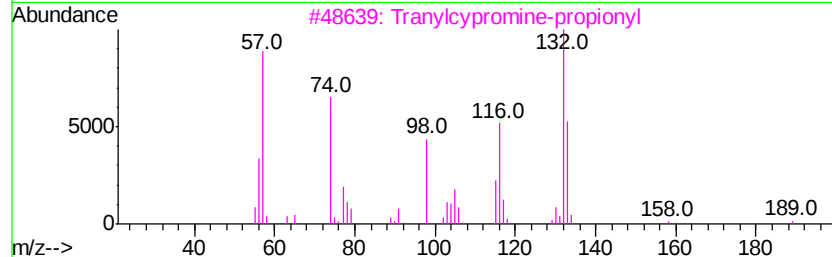
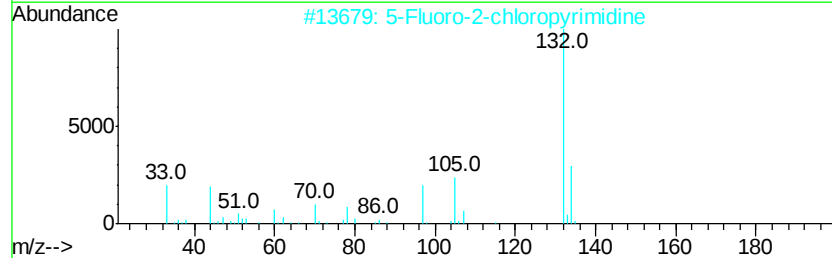
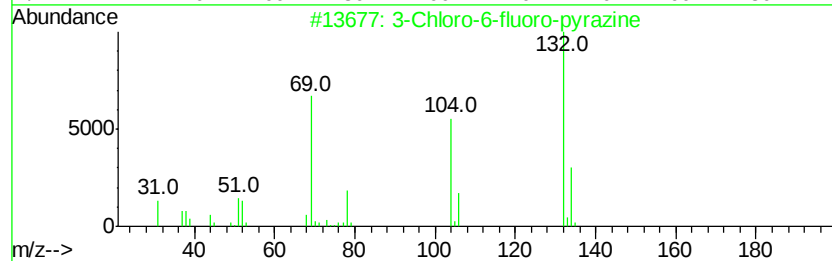
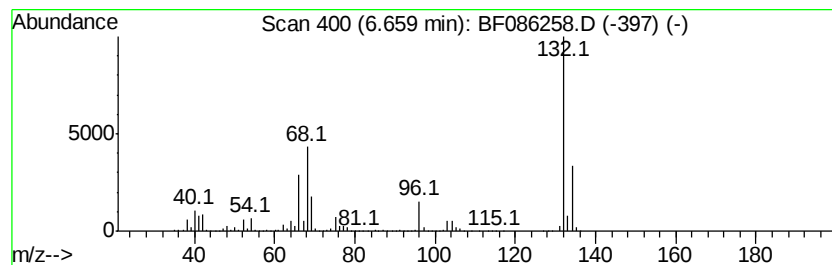
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	70.50 ng	5914190	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9	
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	



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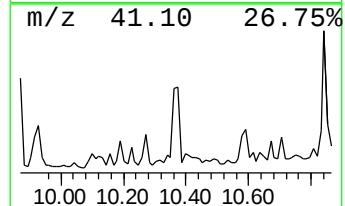
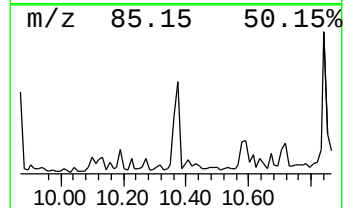
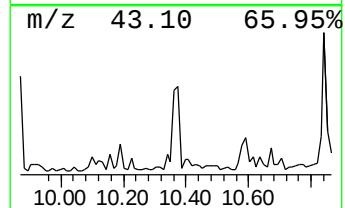
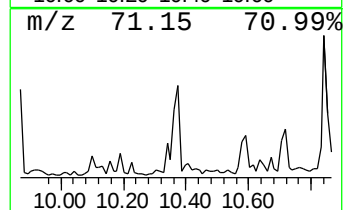
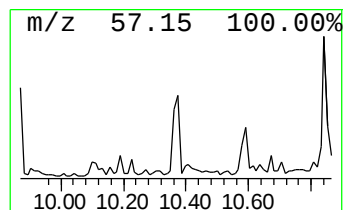
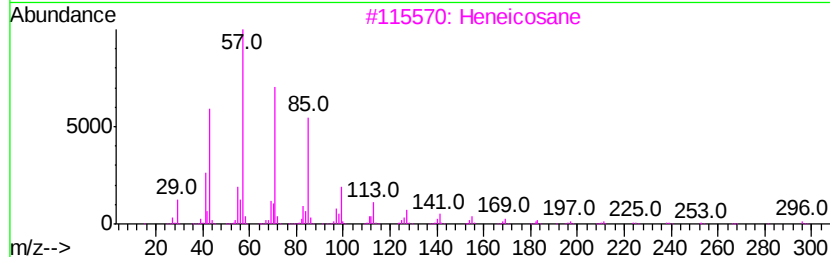
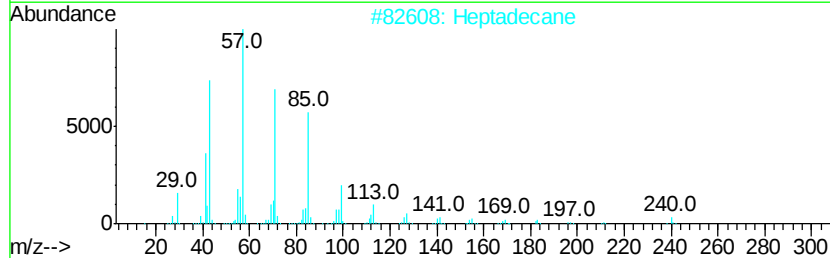
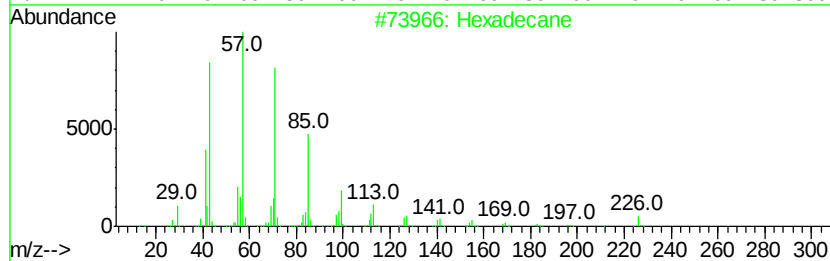
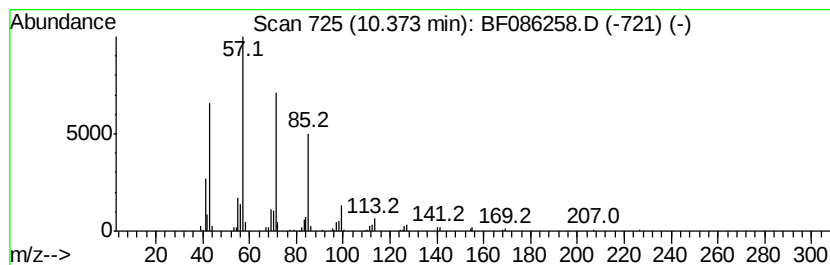
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	2.45 ng	314685	Acenaphthene-d10	9.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	93
2	Heptadecane		240	C17H36	000629-78-7	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Pentadecane		212	C15H32	000629-62-9	86
5	Tetradecane		198	C14H30	000629-59-4	86



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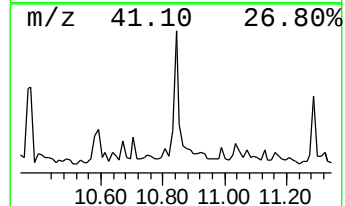
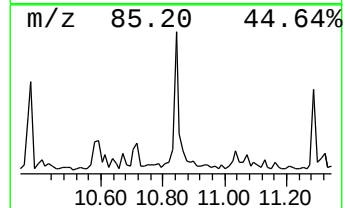
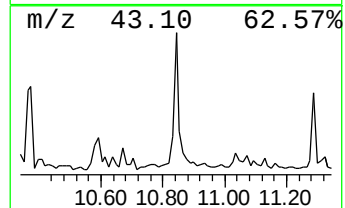
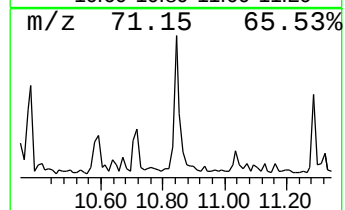
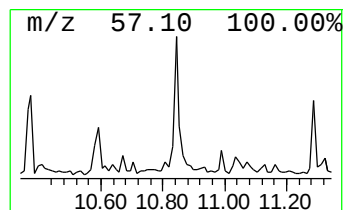
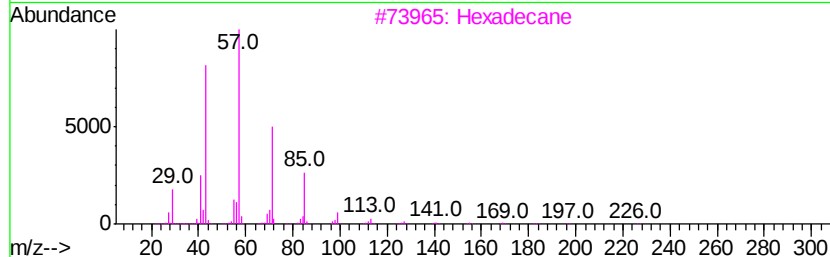
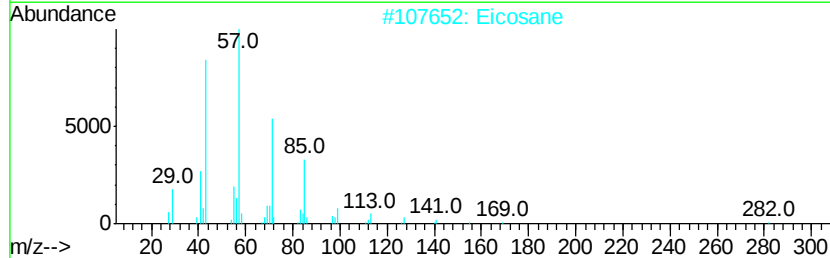
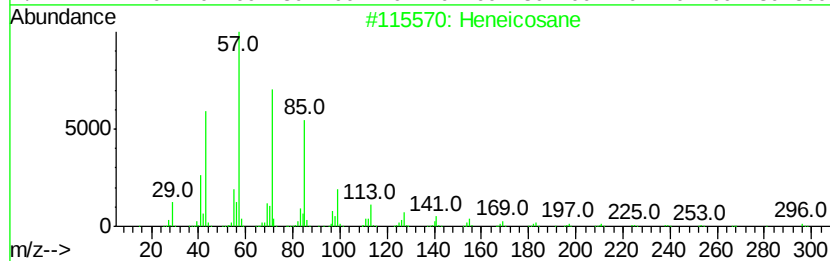
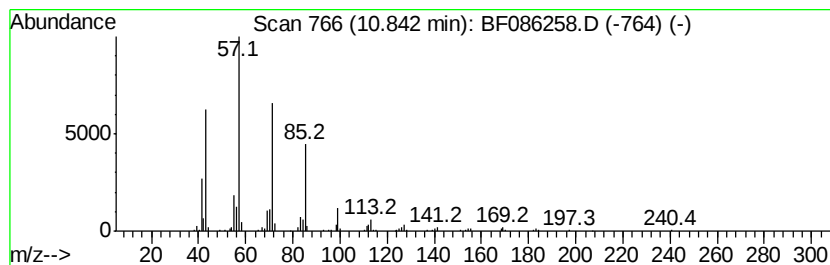
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Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	3.27 ng	392648	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Eicosane		282	C20H42	000112-95-8	90
3	Hexadecane		226	C16H34	000544-76-3	83
4	Nonane, 5-butyl-		184	C13H28	017312-63-9	81
5	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
Data File : BF086258.D
Acq On : 16 Apr 2016 11:39
Operator : UM/SJ
Sample : H2471-02
Misc :
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ClientSampleId :
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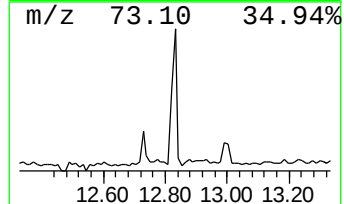
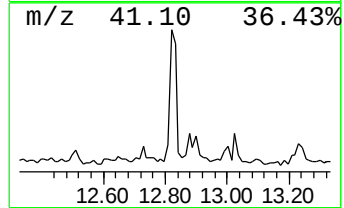
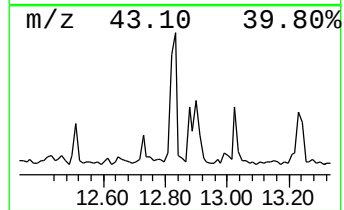
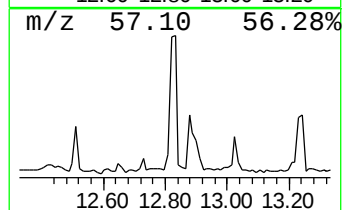
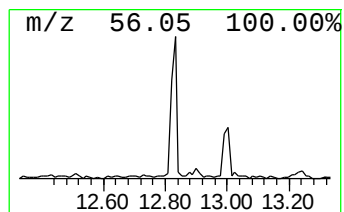
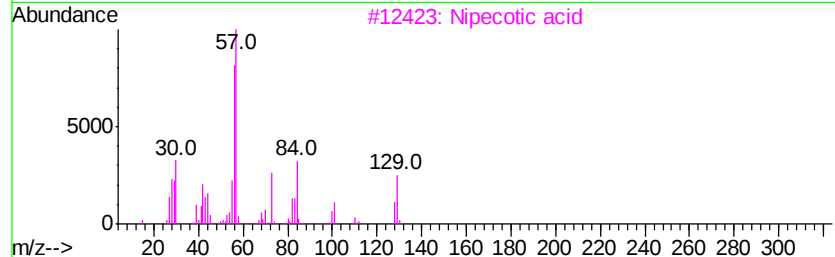
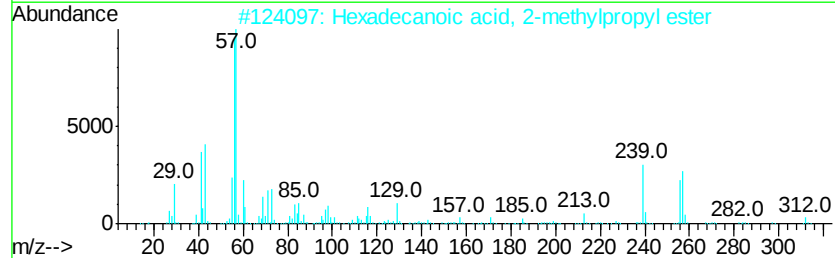
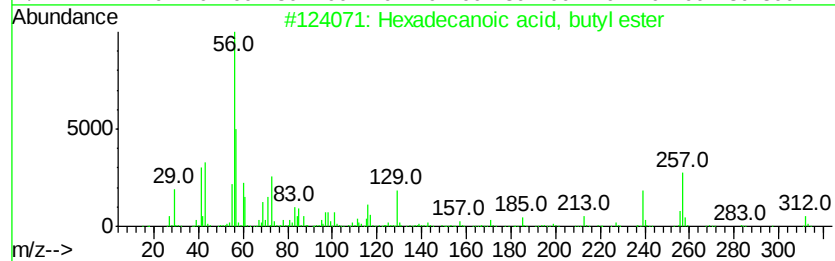
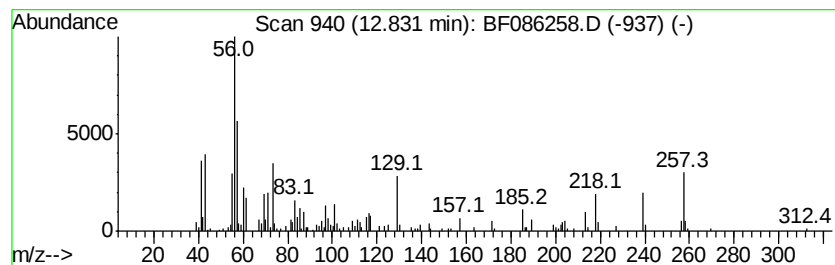
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	4.86 ng	405190	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	93
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	40
3		Nipecotic acid	129	C6H11NO2	000498-95-3	38
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	25
5		Cyclohexanamine	99	C6H13N	000108-91-8	25



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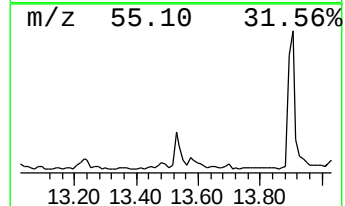
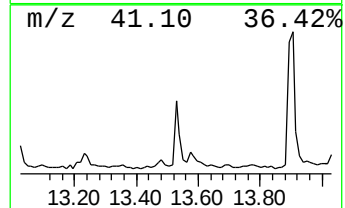
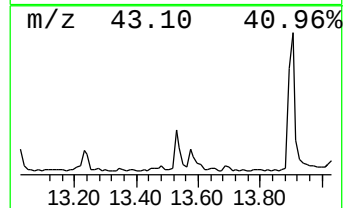
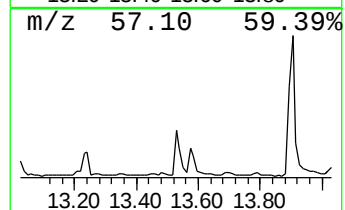
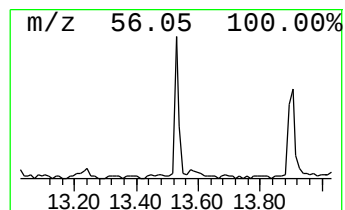
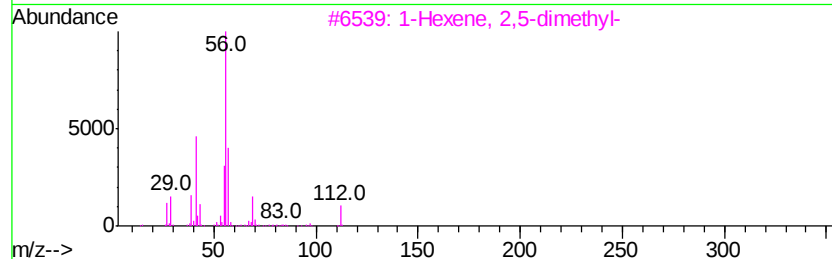
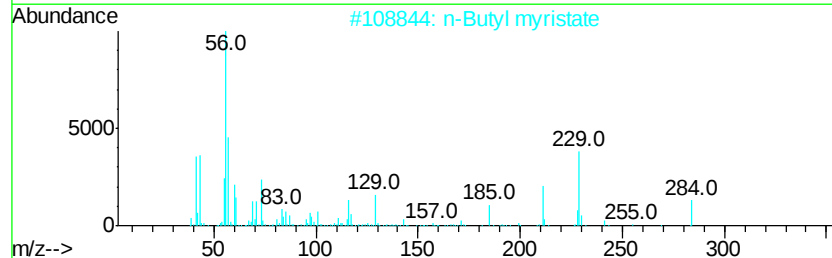
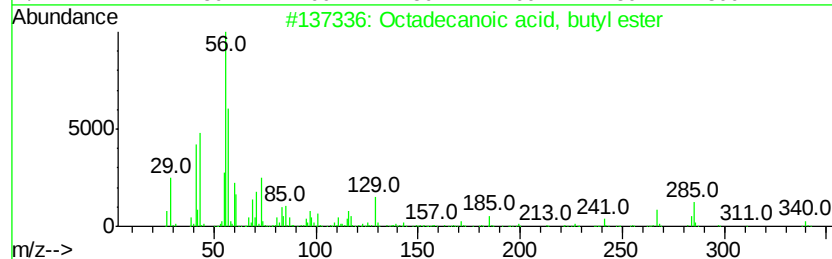
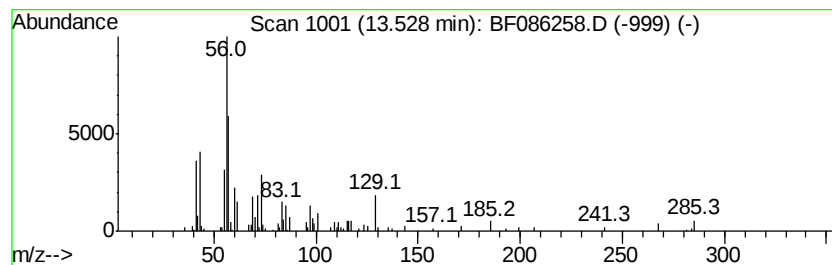
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.13 ng	177534	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
4		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
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Acq On : 16 Apr 2016 11:39
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Sample : H2471-02
Misc :
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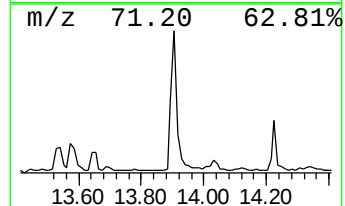
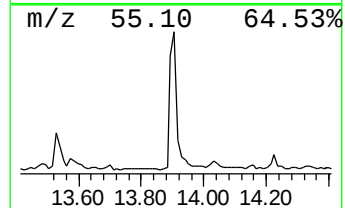
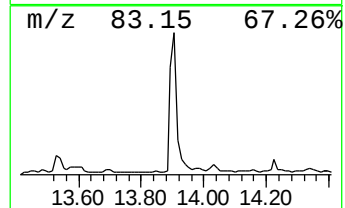
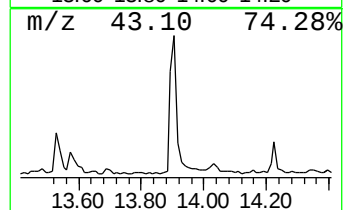
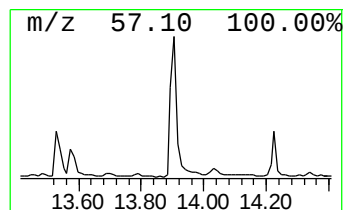
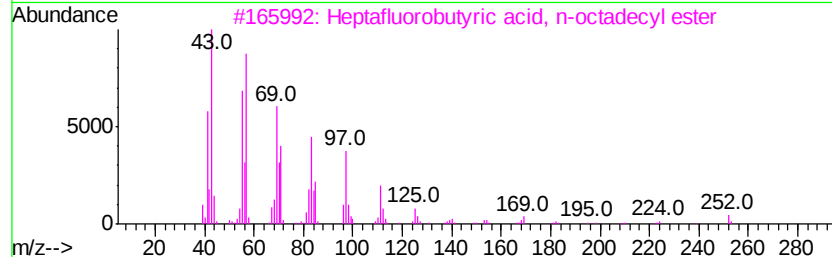
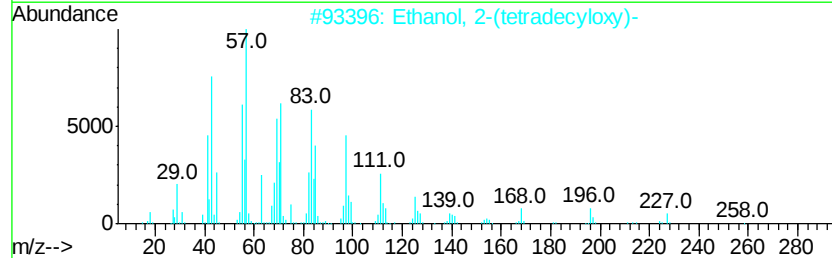
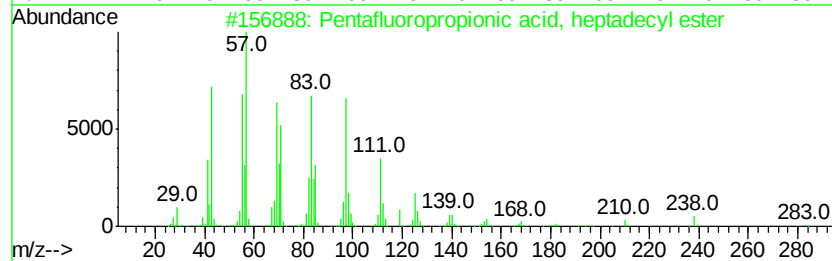
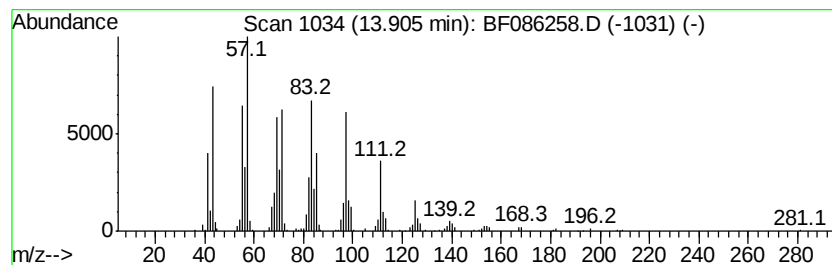
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	6.94 ng	578553	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	83
5		17-Pentatriacontene	491	C35H70	006971-40-0	83



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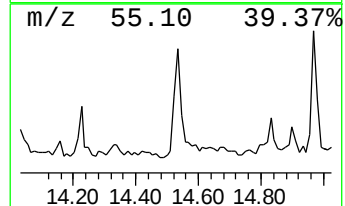
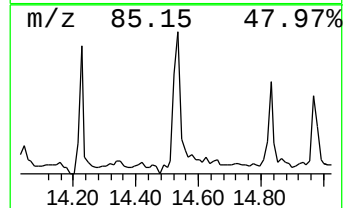
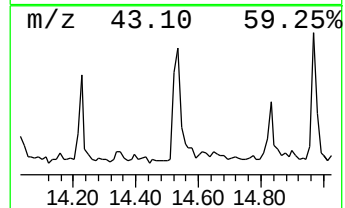
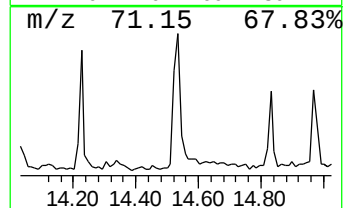
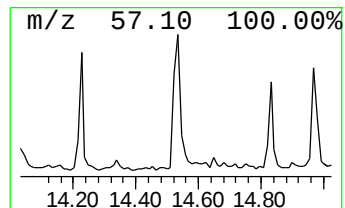
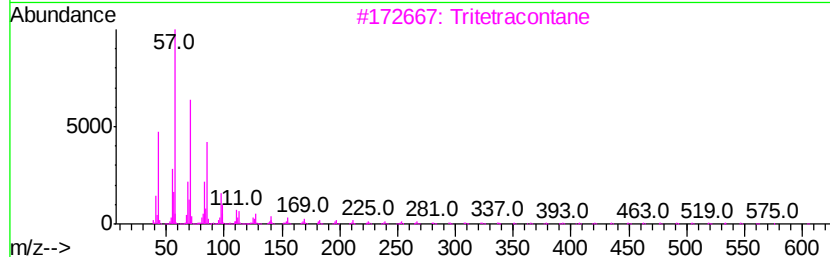
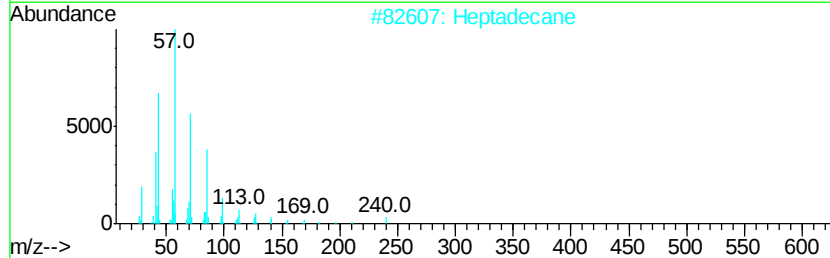
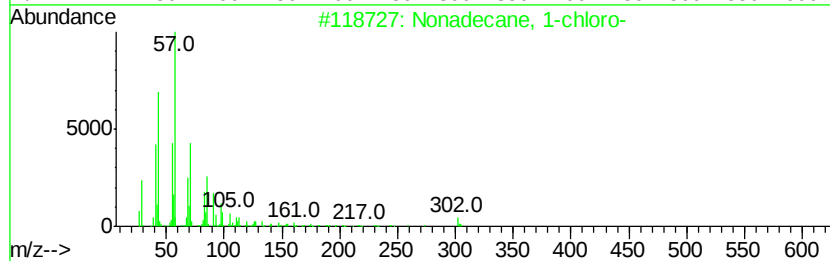
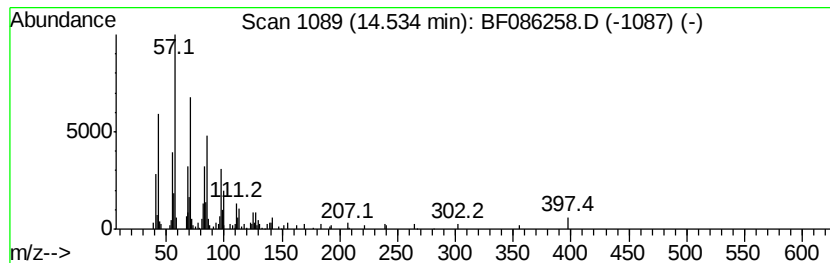
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane, 1-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.17 ng	181020	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	95
2		Heptadecane	240	C17H36	000629-78-7	86
3		Tritetracontane	605	C43H88	007098-21-7	83
4		Eicosane	282	C20H42	000112-95-8	64
5		Octadecane	254	C18H38	000593-45-3	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
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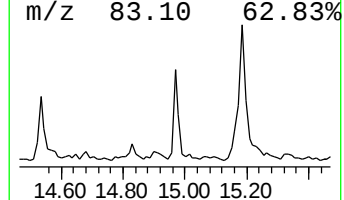
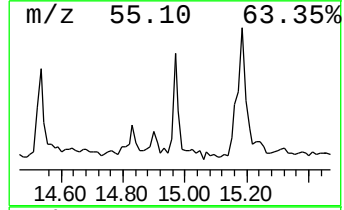
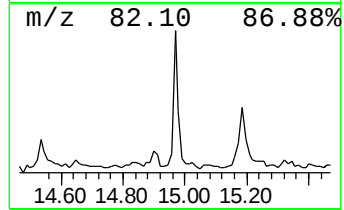
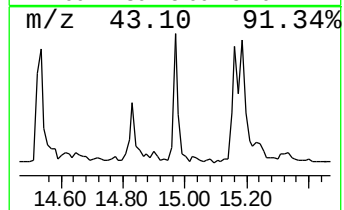
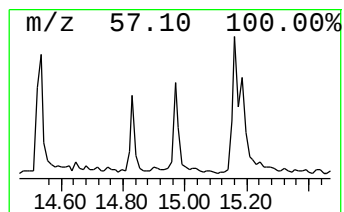
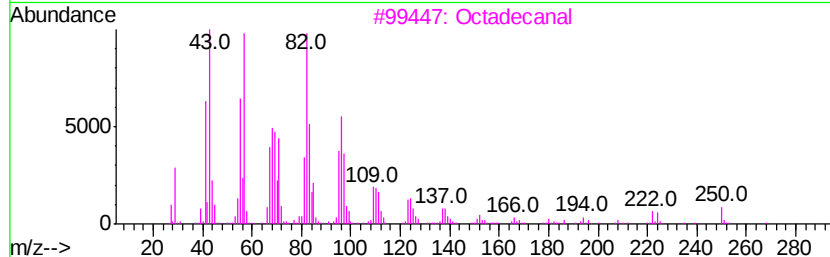
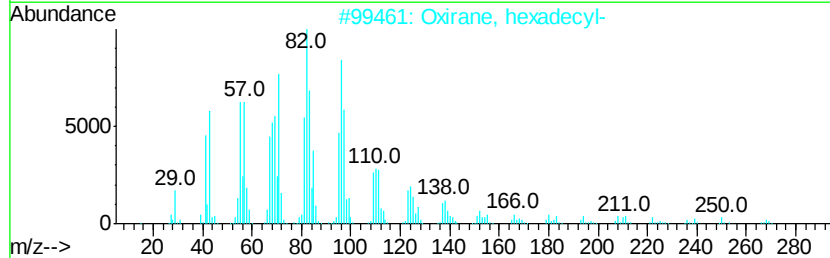
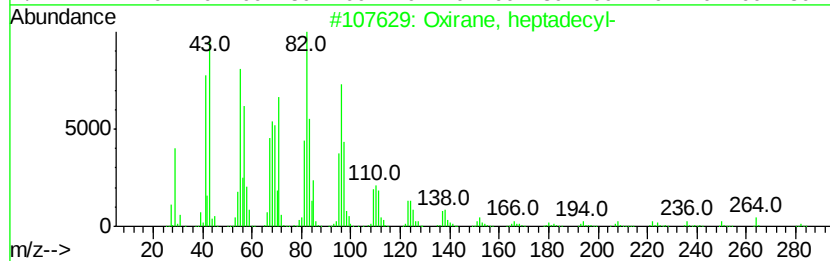
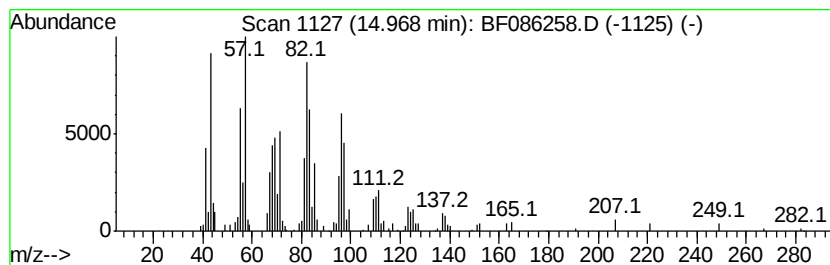
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxirane, heptadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.12 ng	143834	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Octadecanal	268	C18H36O	000638-66-4	72
4		17-Octadecenal	266	C18H34O	056554-86-0	72
5		1,19-Eicosadiene	278	C20H38	014811-95-1	68



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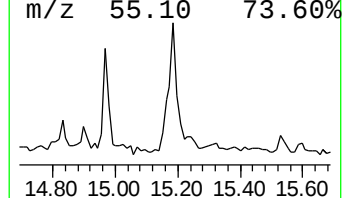
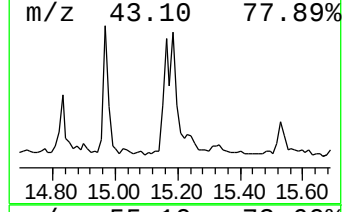
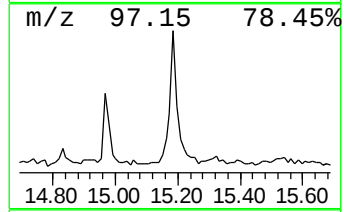
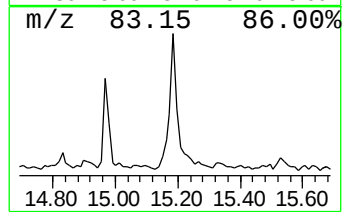
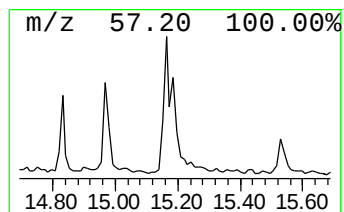
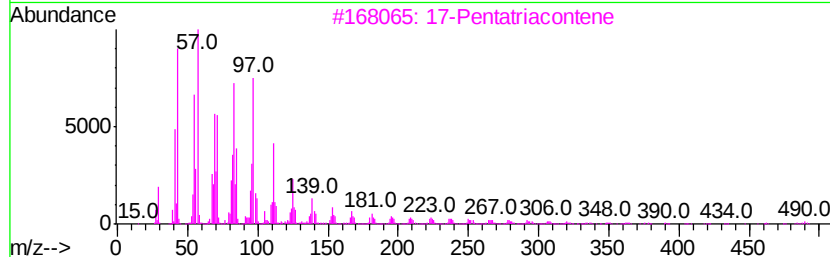
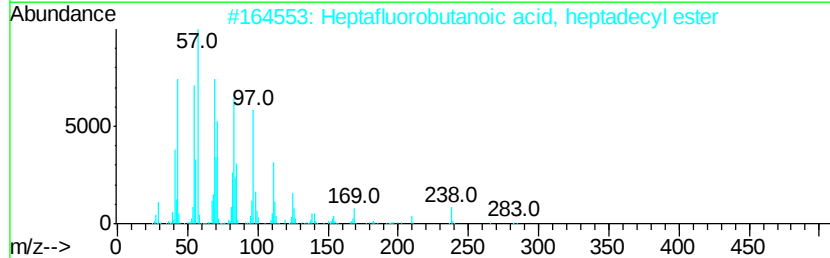
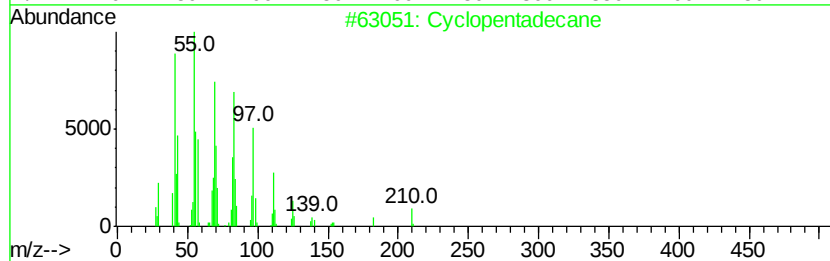
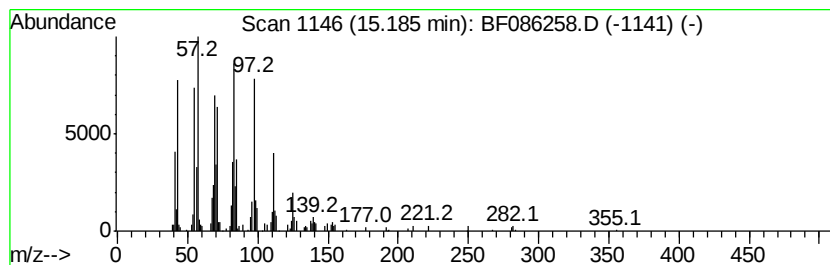
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	4.65 ng	315398	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	97
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5		1-Docosene	308	C22H44	001599-67-3	90



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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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2-Pentanone, 4-hy...	5.09	4.8	ng	400732	1	6.89	1677900	20.0
unknown6.66	6.66	70.5	ng	5914190	1	6.89	1677900	20.0
Hexadecane	10.37	2.5	ng	314685	3	9.93	2564180	20.0
Heneicosane	10.84	3.3	ng	392648	4	11.41	2403170	20.0
Hexadecanoic acid...	12.83	4.9	ng	405190	5	14.04	1666590	20.0
Octadecanoic acid...	13.53	2.1	ng	177534	5	14.04	1666590	20.0
Pentafluoropropio...	13.91	6.9	ng	578553	5	14.04	1666590	20.0
Nonadecane, 1-chl...	14.53	2.2	ng	181020	5	14.04	1666590	20.0
Oxirane, heptadecyl-	14.97	2.1	ng	143834	6	15.48	1355120	20.0
Cyclopentadecane	15.19	4.7	ng	315398	6	15.48	1355120	20.0