

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
 Data File : BF082727.D
 Acq On : 5 Nov 2015 14:09
 Operator : UM/IZ
 Sample : G4241-14
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10(18-20)

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-BF103015.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	5.059	256	260	268	rVB	2006169	3080135	43.48%	4.752%
2	5.470	293	296	299	rBV	4388744	6018358	84.95%	9.285%
3	6.499	382	386	388	rVB	5138442	5801005	81.88%	8.949%
4	6.636	395	398	400	rBV	6154158	6670949	94.16%	10.291%
5	6.864	415	418	420	rBV	1313872	1219472	17.21%	1.881%
6	7.024	429	432	434	rVB	4701091	4955467	69.95%	7.645%
7	7.425	464	467	469	rBV	3497494	3786826	53.45%	5.842%
8	8.145	528	530	533	rBV	1535449	1507925	21.28%	2.326%
9	9.105	612	614	617	rBV	111143	101326	1.43%	0.156%
10	9.230	622	625	627	rBV	6953417	7084459	100.00%	10.929%
11	9.322	630	633	634	rBV	70873	85263	1.20%	0.132%
12	9.619	656	659	661	rBV	1270050	1144733	16.16%	1.766%
13	9.848	677	679	681	rVB	159201	131682	1.86%	0.203%
14	9.905	681	684	686	rBV	1951755	1929441	27.23%	2.977%
15	10.351	721	723	724	rVB	174441	169303	2.39%	0.261%
16	10.568	739	742	745	rBV	128205	165313	2.33%	0.255%
17	10.693	749	753	755	rVV	4329851	4936617	69.68%	7.616%
18	10.819	762	764	768	rVB	315882	427435	6.03%	0.659%
19	11.265	801	803	805	rBV	290162	255770	3.61%	0.395%
20	11.299	805	806	808	rVB	128959	104102	1.47%	0.161%
21	11.379	811	813	816	rVV	1697125	1817214	25.65%	2.803%
22	11.436	816	818	821	rVB2	35588	73091	1.03%	0.113%
23	11.688	838	840	842	rBV	175781	208995	2.95%	0.322%
24	11.859	852	855	859	rBV6	30542	106076	1.50%	0.164%
25	11.916	859	860	862	rBV	191867	274077	3.87%	0.423%
26	12.099	874	876	878	rVB	217099	172552	2.44%	0.266%
27	12.488	908	910	912	rVB	179121	143656	2.03%	0.222%
28	12.705	927	929	931	rBV	80653	91517	1.29%	0.141%
29	12.808	936	938	939	rVB	114121	125607	1.77%	0.194%
30	12.865	941	943	947	rVB	107305	157679	2.23%	0.243%
31	12.979	950	953	955	rVB	6363190	7046002	99.46%	10.870%
32	13.219	972	974	975	rVB	110028	121591	1.72%	0.188%
33	13.459	989	995	998	rBV	197503	334404	4.72%	0.516%
34	13.505	998	999	1001	rVV	77869	97779	1.38%	0.151%

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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-BF103015.M
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35	13.562	1001	1004	1005	rVB	103903	106965	1.51%	0.165%
36	13.882	1029	1032	1038	rBV2	346628	560453	7.91%	0.865%
37	14.031	1042	1045	1047	rVV	1313790	1879867	26.54%	2.900%
38	14.214	1059	1061	1063	rBV	118549	122256	1.73%	0.189%
39	14.534	1087	1089	1094	rVB	124479	152696	2.16%	0.236%
40	14.842	1115	1116	1119	rVB	67439	100401	1.42%	0.155%
41	14.922	1120	1123	1125	rBV	73731	80374	1.13%	0.124%
42	15.174	1143	1145	1148	rVB	60102	81699	1.15%	0.126%
43	15.482	1169	1172	1175	rBV	937382	1389726	19.62%	2.144%

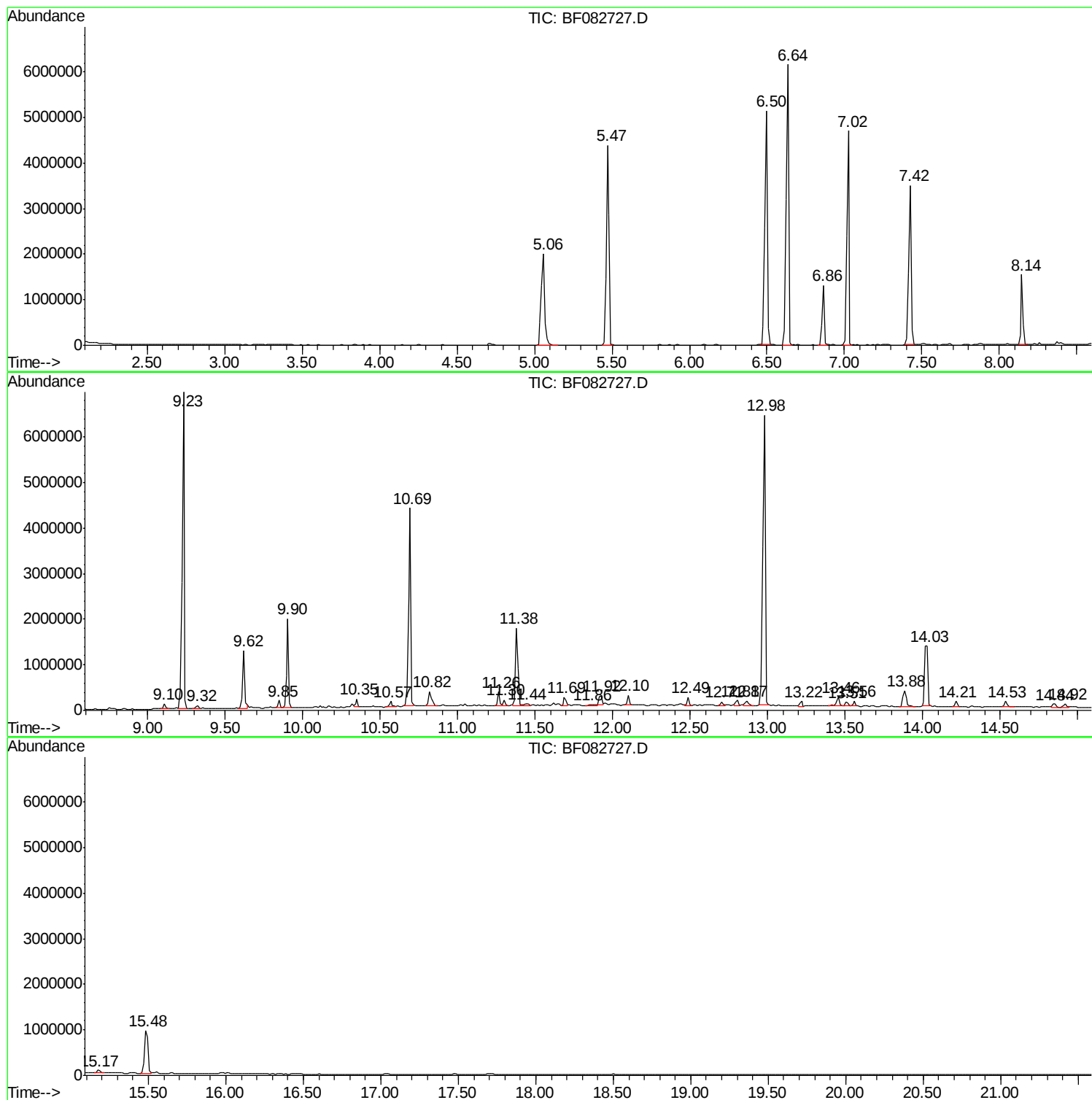
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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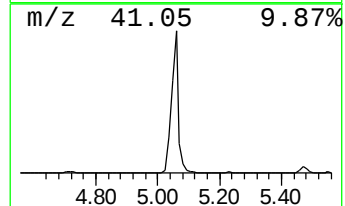
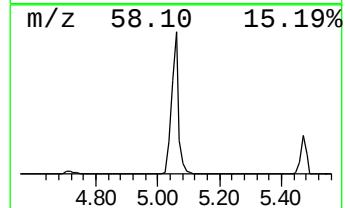
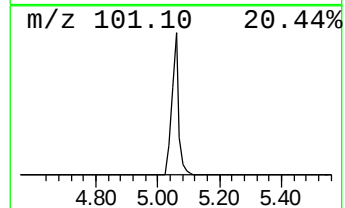
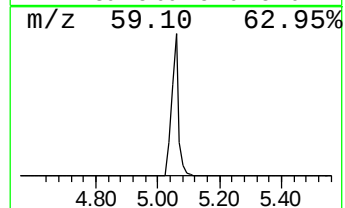
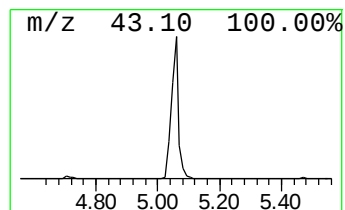
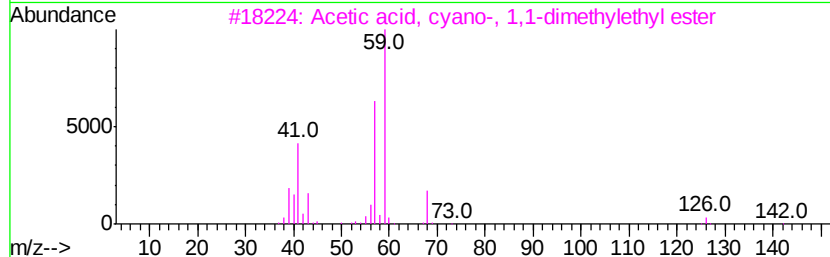
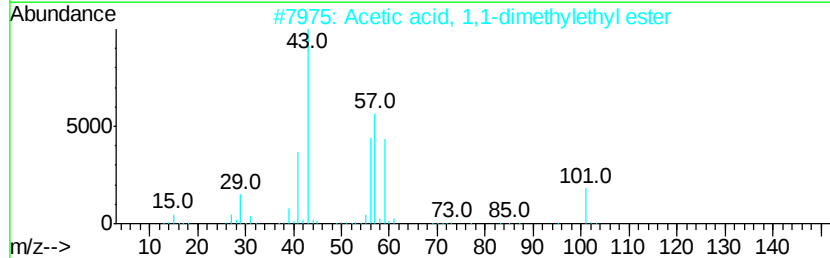
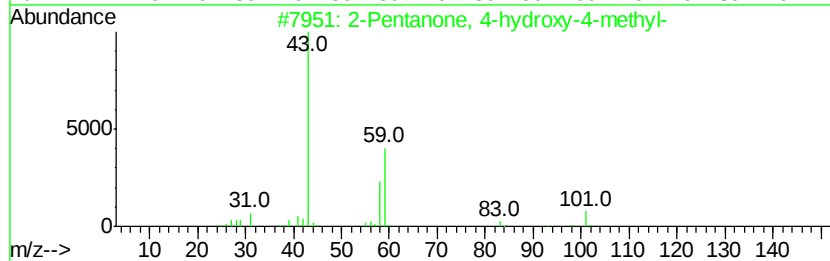
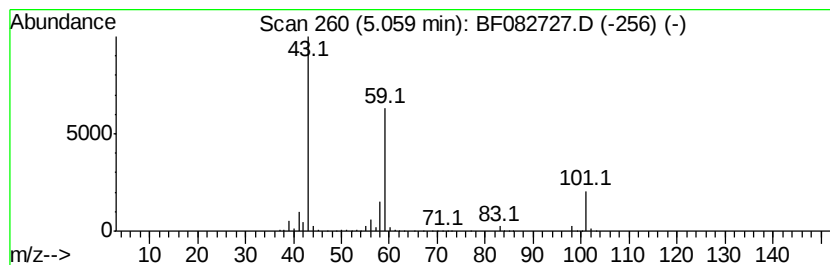
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	50.52 ng	3080140	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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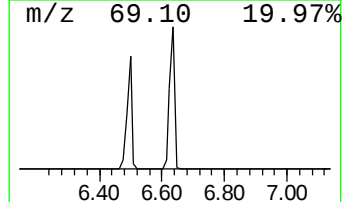
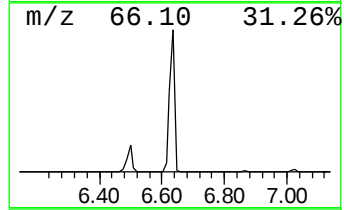
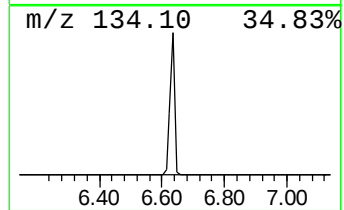
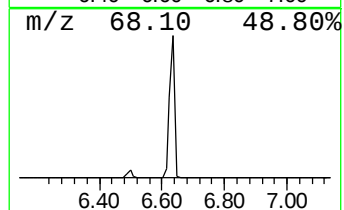
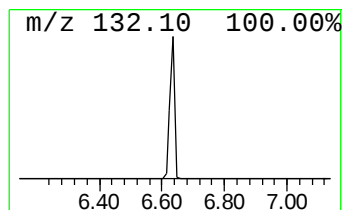
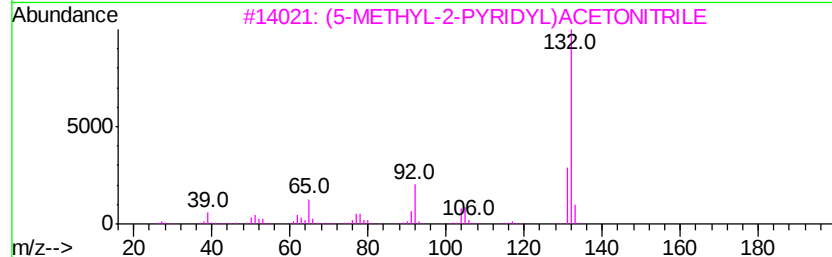
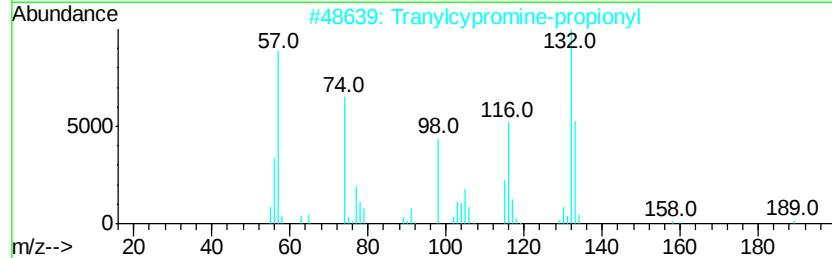
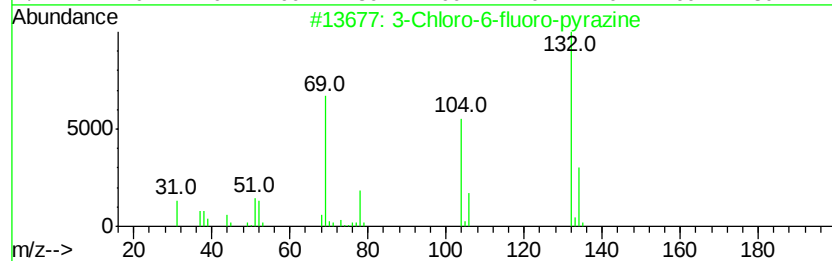
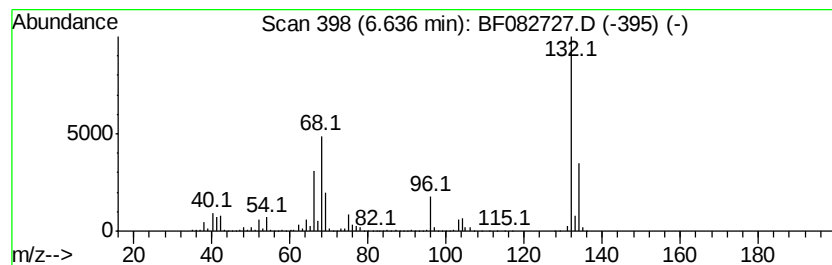
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	109.41 ng	6670950	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	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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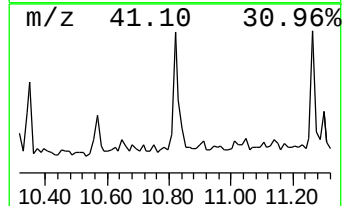
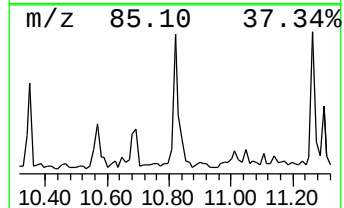
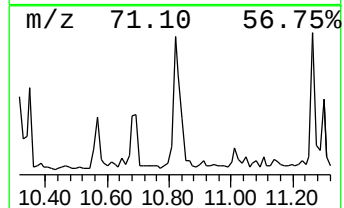
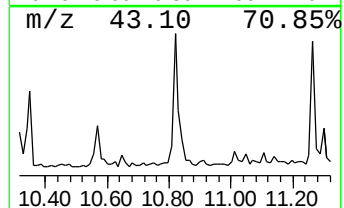
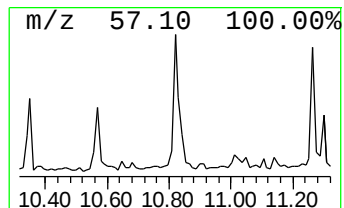
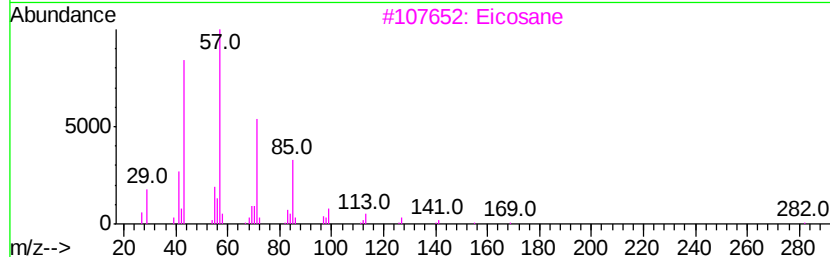
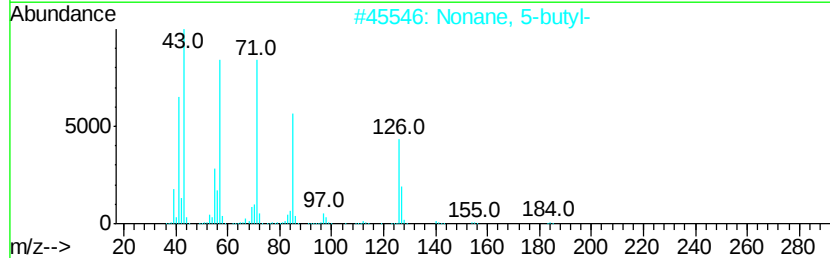
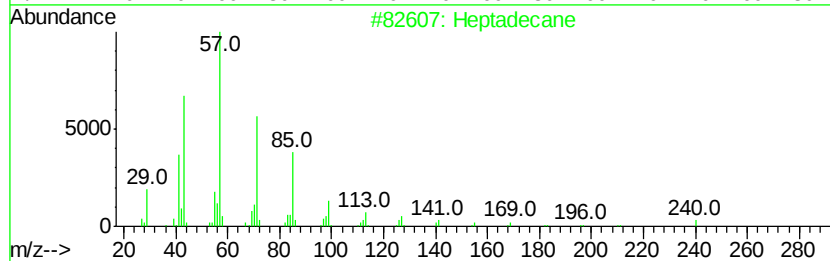
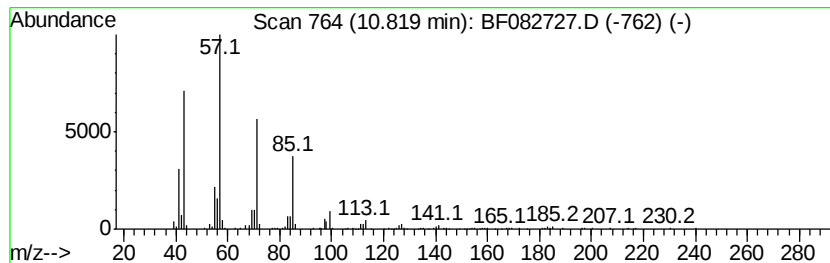
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	4.70 ng	427435	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Nonane, 5-butyl-	184	C13H28	017312-63-9	92
3	Eicosane	282	C20H42	000112-95-8	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetracosane	338	C24H50	000646-31-1	86



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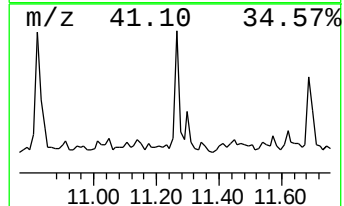
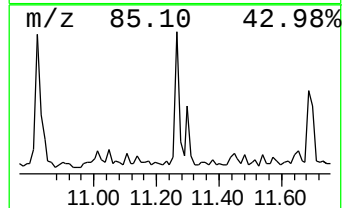
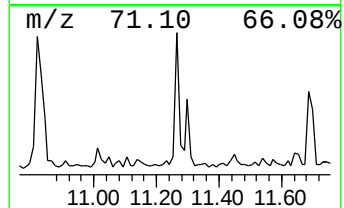
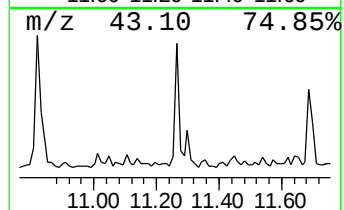
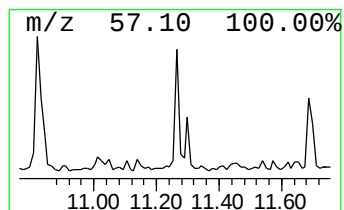
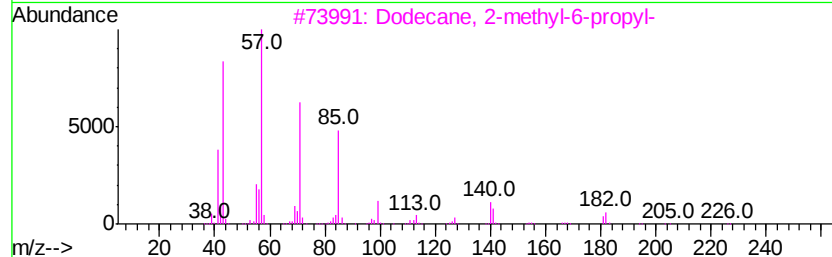
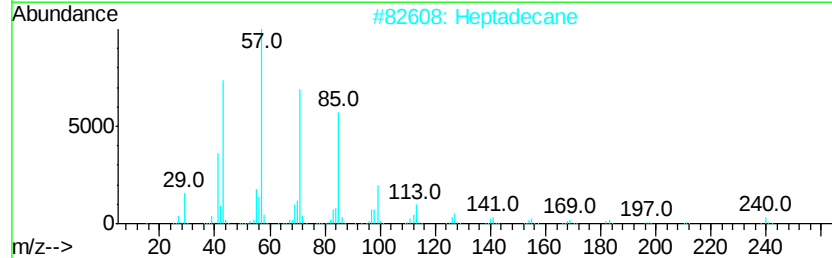
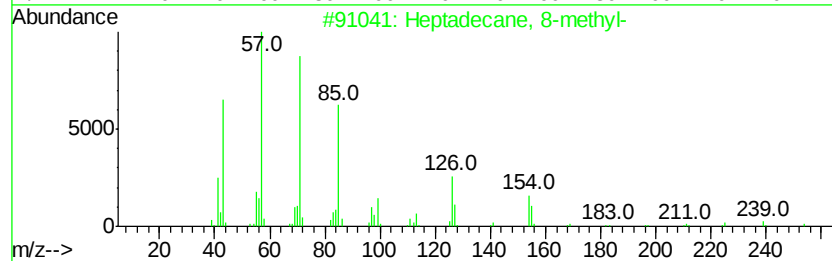
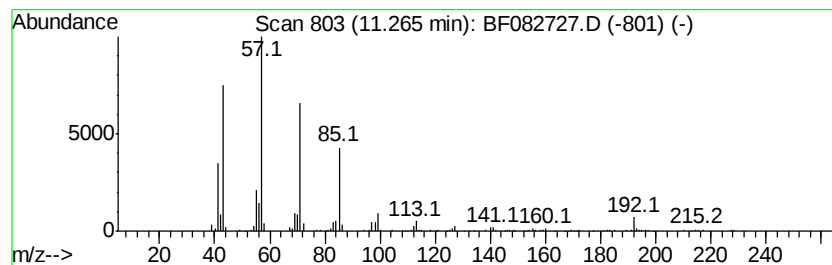
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane, 8-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.81 ng	255770	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 8-methyl-	254	C18H38	013287-23-5	83
2		Heptadecane	240	C17H36	000629-78-7	83
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4		Undecane, 5-methyl-	170	C12H26	001632-70-8	76
5		Decane, 3-methyl-	156	C11H24	013151-34-3	74



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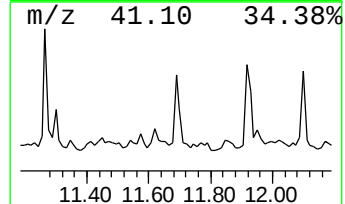
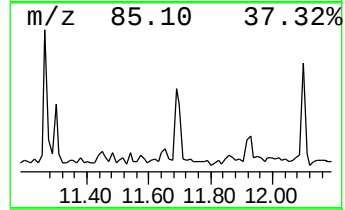
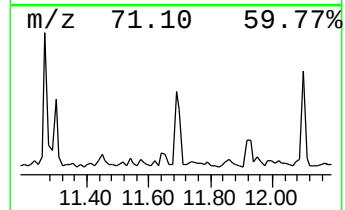
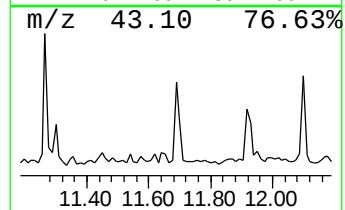
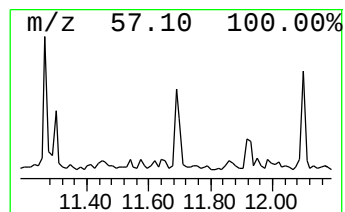
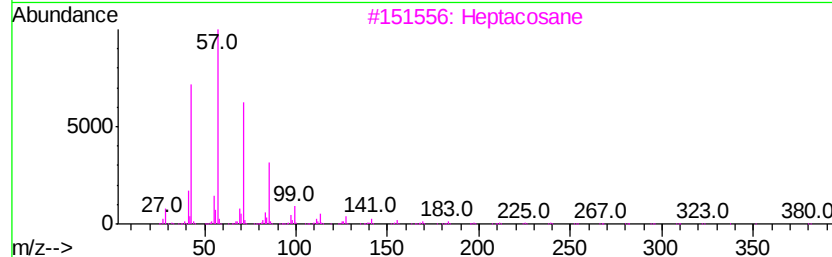
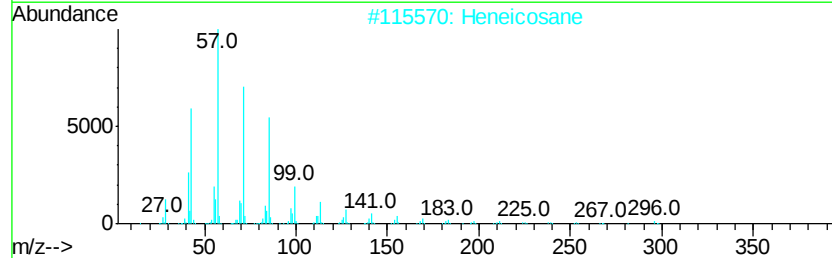
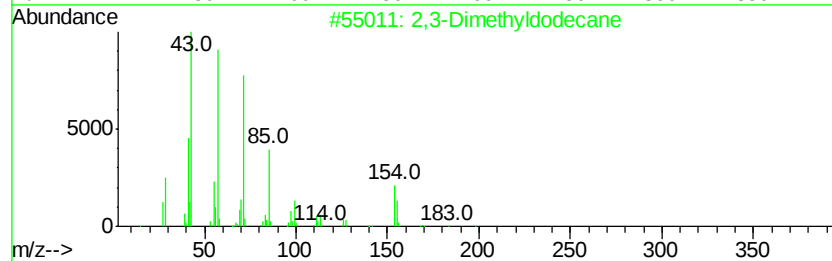
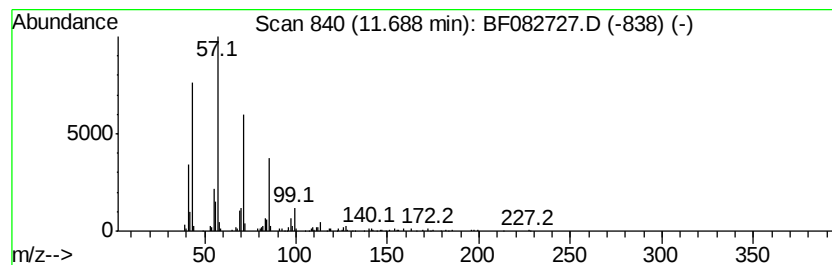
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Peak Number 6 2,3-Dimethyldodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.30 ng	208995	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Dimethyldodecane	198	C14H30	006117-98-2	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptacosane	380	C27H56	000593-49-7	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082727.D
Acq On : 5 Nov 2015 14:09
Operator : UM/IZ
Sample : G4241-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10(18-20)

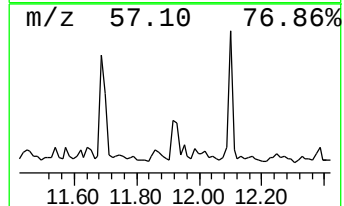
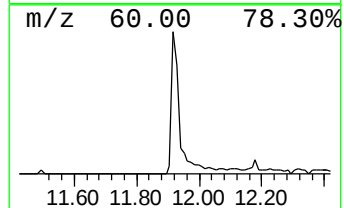
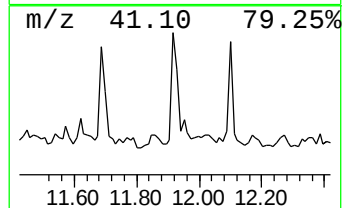
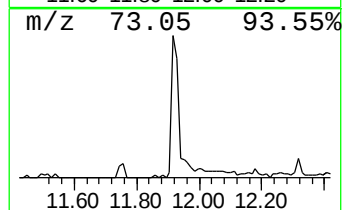
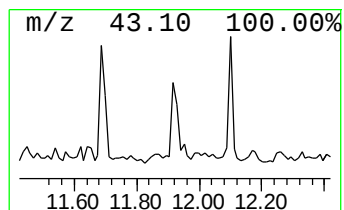
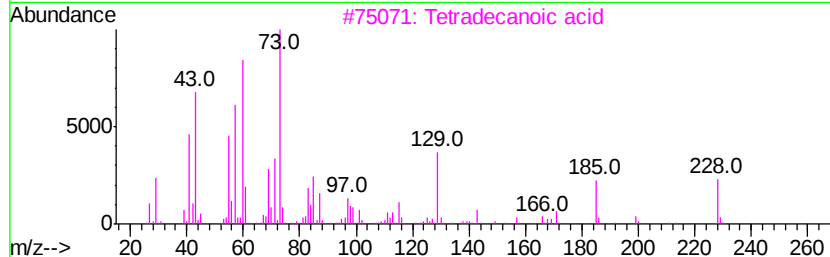
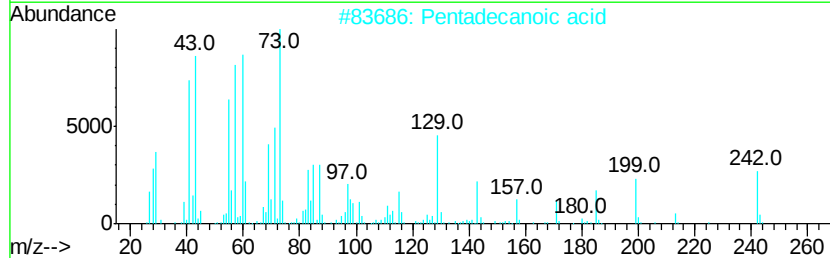
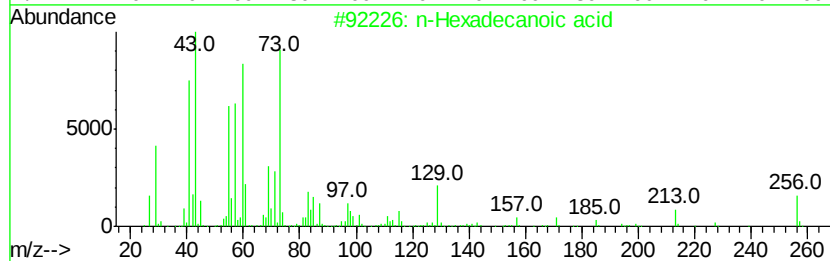
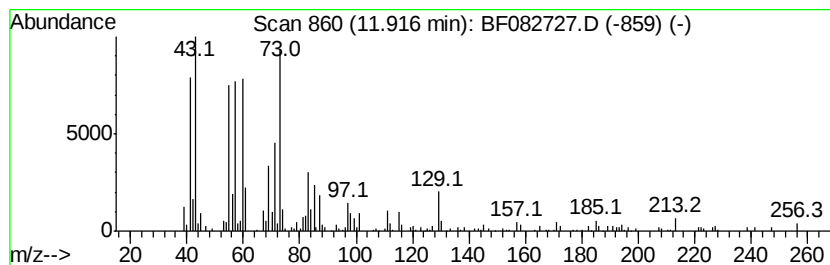
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.02 ng	274077	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93	
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59	
4	Nonanoic acid	158	C9H18O2	000112-05-0	50	
5	Undecanoic acid	186	C11H22O2	000112-37-8	50	



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Operator : UM/IZ
Sample : G4241-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

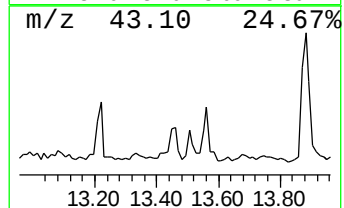
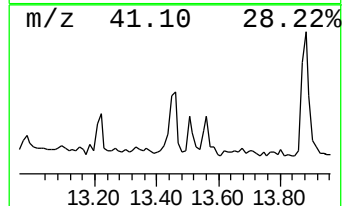
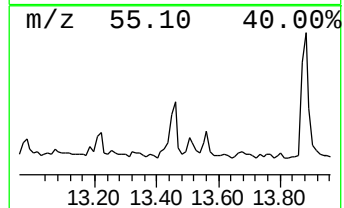
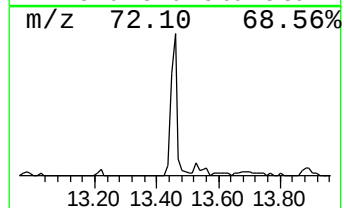
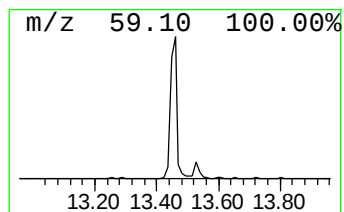
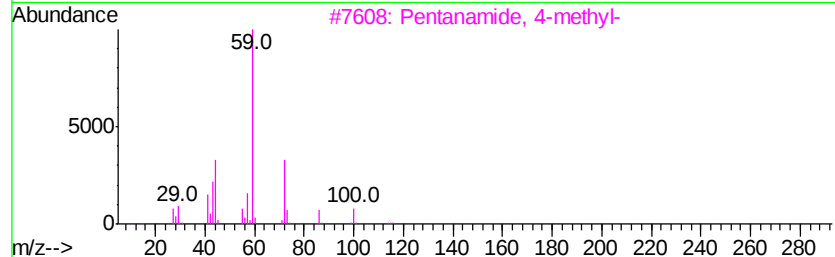
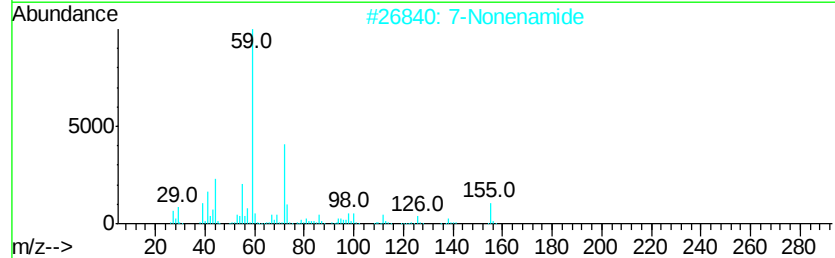
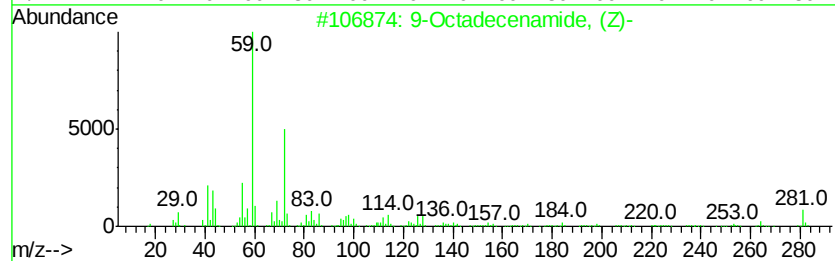
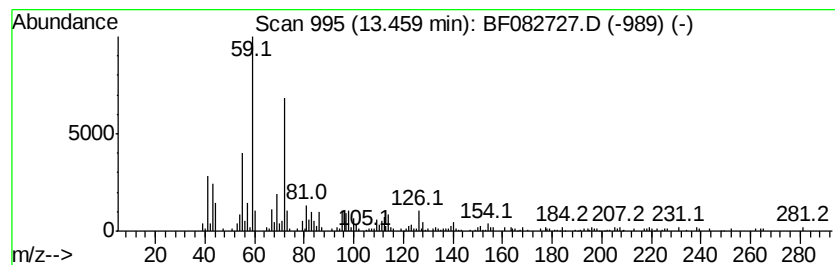
Instrument :
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ClientSampleId :
SB-10(18-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.46	3.56 ng	334404	Chrysene-d12		14.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Octanamide	143	C8H17NO	000629-01-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082727.D
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Operator : UM/IZ
Sample : G4241-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10(18-20)

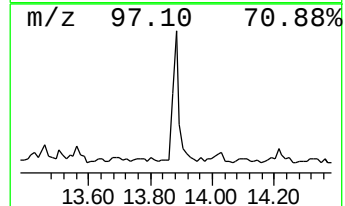
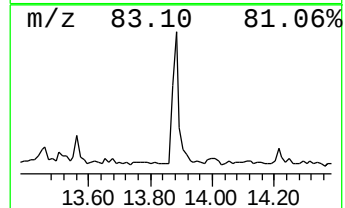
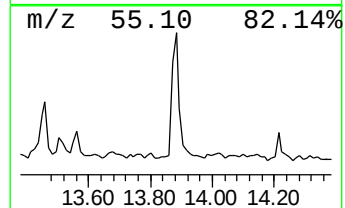
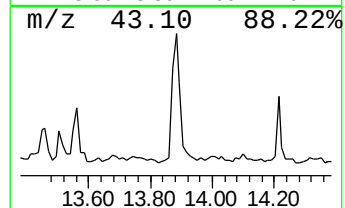
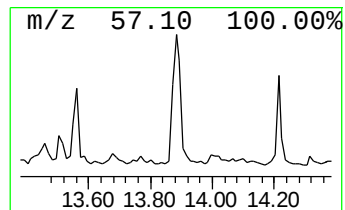
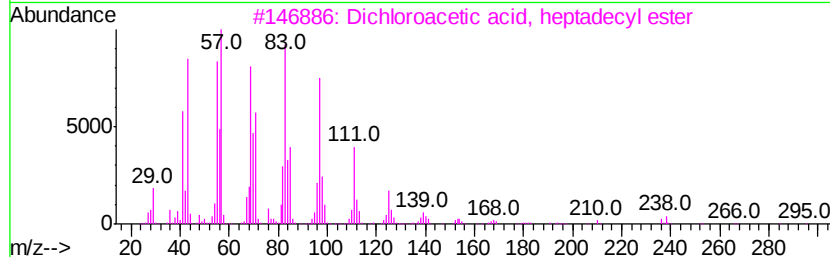
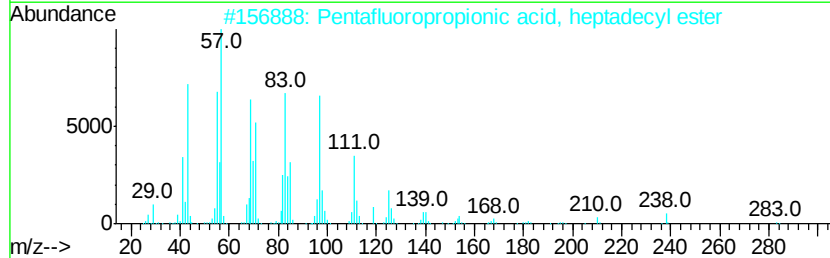
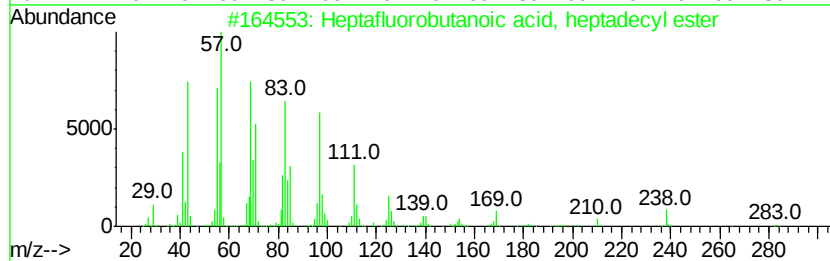
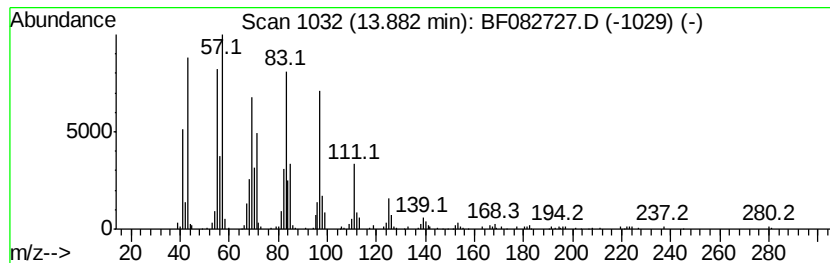
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	5.96 ng	560453	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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Operator : UM/IZ
Sample : G4241-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10(18-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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...	5.06	50.5	ng	3080140	1	6.86	1219470	20.0
unknown6.64	6.64	109.4	ng	6670950	1	6.86	1219470	20.0
Heptadecane	10.82	4.7	ng	427435	4	11.38	1817210	20.0
Heptadecane, 8-me...	11.26	2.8	ng	255770	4	11.38	1817210	20.0
2,3-Dimethyldodecane	11.69	2.3	ng	208995	4	11.38	1817210	20.0
n-Hexadecanoic acid	11.92	3.0	ng	274077	4	11.38	1817210	20.0
9-Octadecenamide,...	13.46	3.6	ng	334404	5	14.03	1879870	20.0
Heptafluorobutano...	13.88	6.0	ng	560453	5	14.03	1879870	20.0