

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
 Data File : BF086699.D
 Acq On : 5 May 2016 1:53
 Operator : UM/SJ
 Sample : H2715-17
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26WARD-2-CS-3(0-10FTBGS)

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-BF050416.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	2.990	77	79	90	rBV	19024	89606	2.15%	0.272%
2	4.201	182	185	194	rBV	215984	325566	7.81%	0.990%
3	4.887	242	245	248	rBV	1184122	1642909	39.43%	4.995%
4	5.333	281	284	286	rBV	1963675	2470079	59.29%	7.510%
5	6.384	373	376	378	rBV	3613105	4166348	100.00%	12.667%
6	6.510	384	387	389	rBV	2650651	3371905	80.93%	10.252%
7	6.579	392	393	395	rVB	67989	50905	1.22%	0.155%
8	6.670	399	401	405	rVB	89169	93795	2.25%	0.285%
9	6.739	405	407	409	rBV	1091073	973825	23.37%	2.961%
10	6.899	418	421	423	rBV	2452901	2977663	71.47%	9.053%
11	7.310	454	457	459	rBV	1851259	2441893	58.61%	7.424%
12	8.019	517	519	522	rBV	757501	1092607	26.22%	3.322%
13	9.105	611	614	616	rBV	3962381	3607456	86.59%	10.968%
14	9.493	646	648	651	rBV	293713	332308	7.98%	1.010%
15	9.722	663	668	670	rBV	83097	96810	2.32%	0.294%
16	9.779	670	673	675	rBV	913865	995787	23.90%	3.028%
17	10.213	710	711	713	rVB	143148	128148	3.08%	0.390%
18	10.431	727	730	734	rBV2	61842	140529	3.37%	0.427%
19	10.556	739	741	744	rBV2	389439	441927	10.61%	1.344%
20	10.613	744	746	748	rVV	90387	121951	2.93%	0.371%
21	10.693	751	753	757	rVB	117430	202577	4.86%	0.616%
22	11.139	790	792	793	rBV	66726	68719	1.65%	0.209%
23	11.253	800	802	807	rBV	877645	899598	21.59%	2.735%
24	11.322	807	808	814	rVB2	29296	46099	1.11%	0.140%
25	12.465	905	908	910	rBV	150574	157835	3.79%	0.480%
26	12.694	924	928	929	rBV	122629	184091	4.42%	0.560%
27	12.842	938	941	943	rBV	2881049	2702720	64.87%	8.217%
28	13.082	958	962	964	rBV	55992	67195	1.61%	0.204%
29	13.425	989	992	993	rBV2	52917	66138	1.59%	0.201%
30	13.745	1018	1020	1025	rBV2	148409	198474	4.76%	0.603%
31	13.882	1029	1032	1039	rBV	826176	1148464	27.57%	3.492%
32	14.065	1046	1048	1050	rBV	48308	56302	1.35%	0.171%
33	14.374	1073	1075	1077	rBV2	42538	64522	1.55%	0.196%
34	14.648	1096	1099	1103	rBV2	141295	264546	6.35%	0.804%

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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-BF050416.M
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35	14.888	1118	1120	1124	rBV	85644	159905	3.84%	0.486%
36	15.162	1142	1144	1147	rVV	45426	61560	1.48%	0.187%
37	15.220	1147	1149	1151	rVV	51960	81399	1.95%	0.247%
38	15.277	1151	1154	1162	rVB	515657	718807	17.25%	2.185%
39	16.637	1270	1273	1276	rVB	100363	179204	4.30%	0.545%

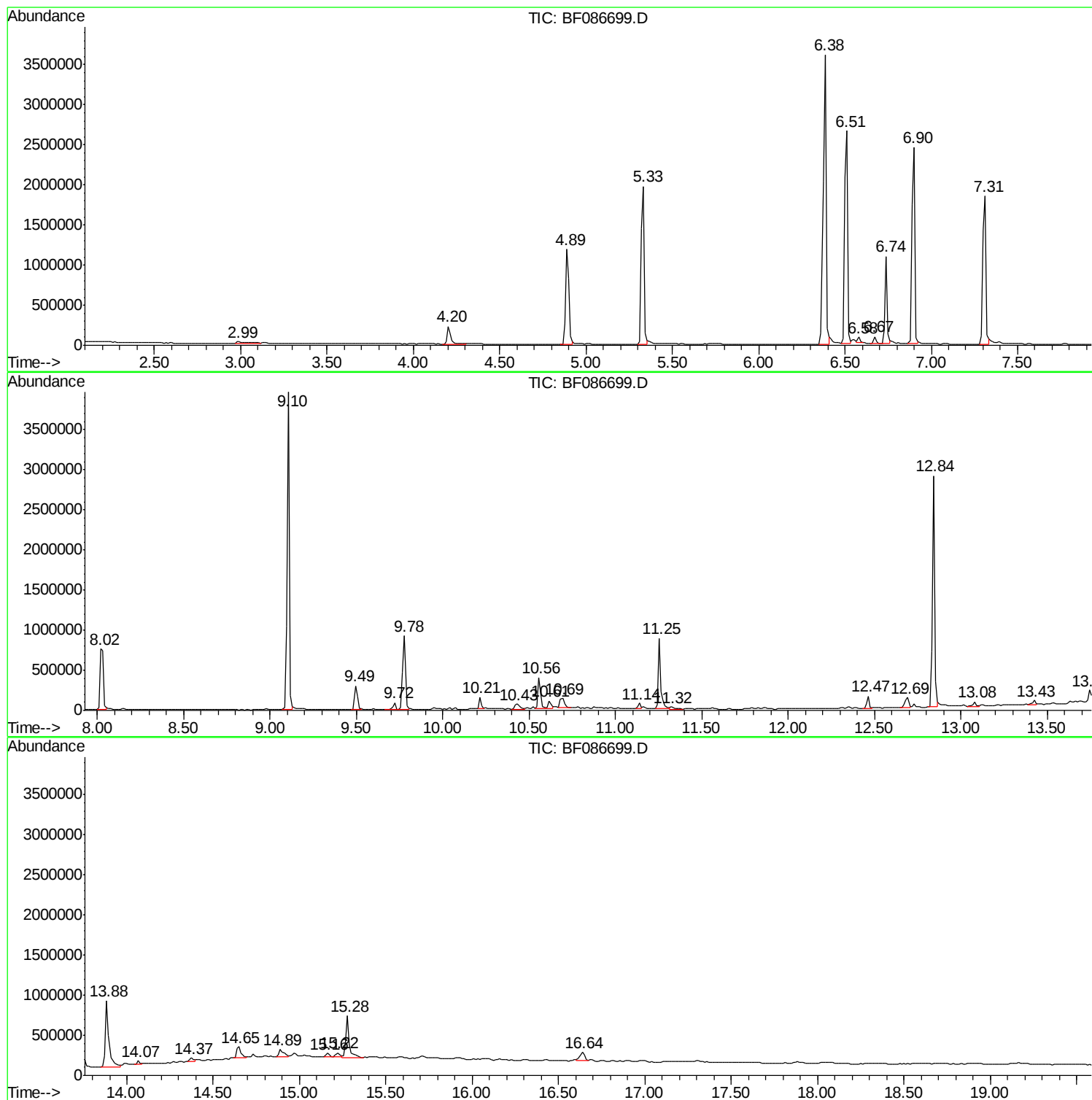
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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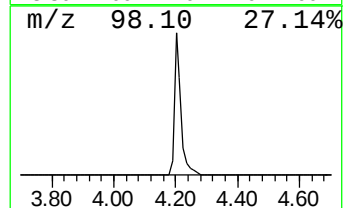
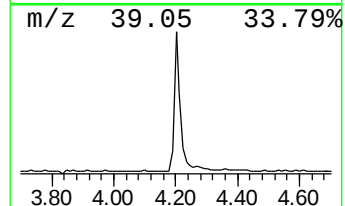
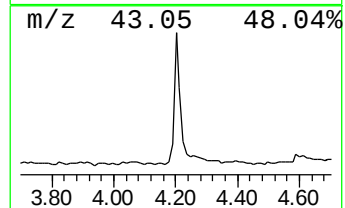
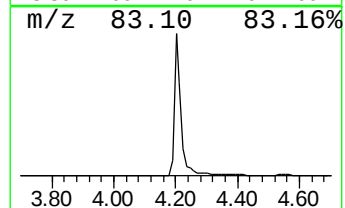
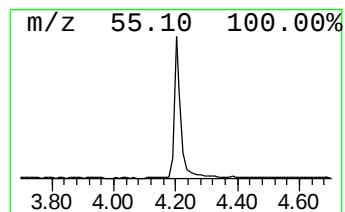
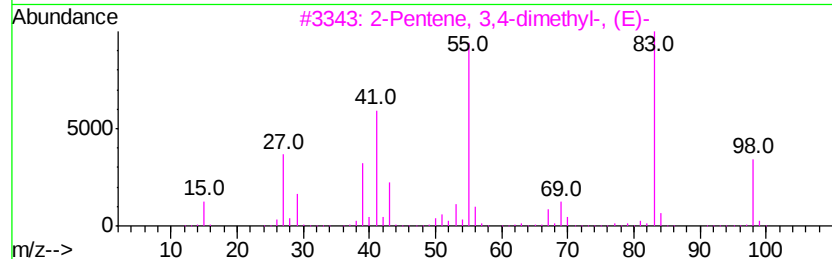
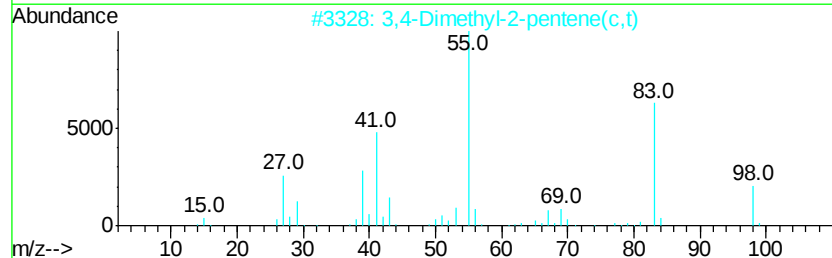
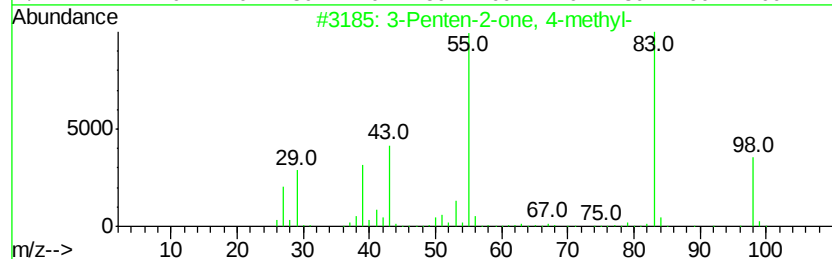
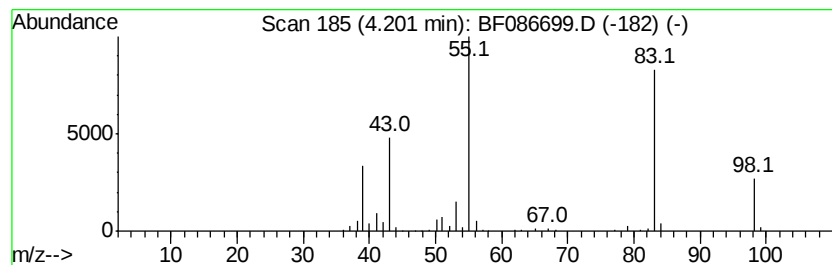
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	13.37 ng	325566	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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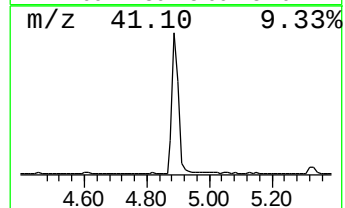
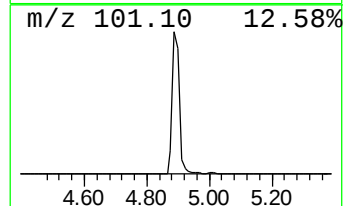
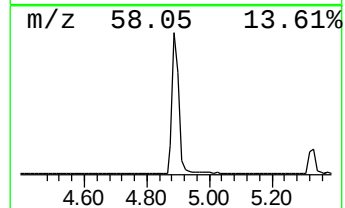
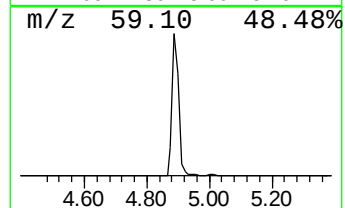
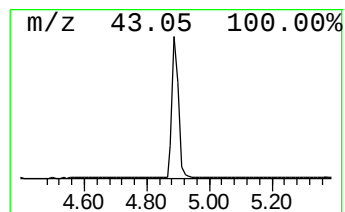
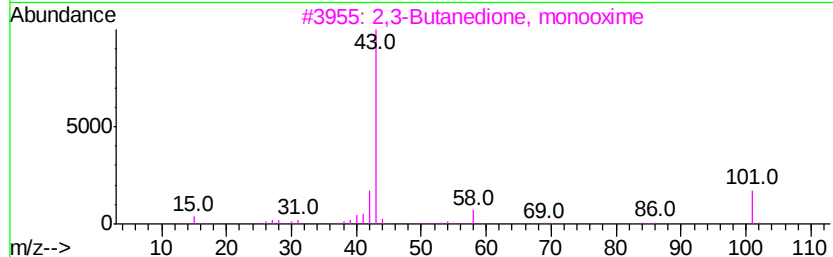
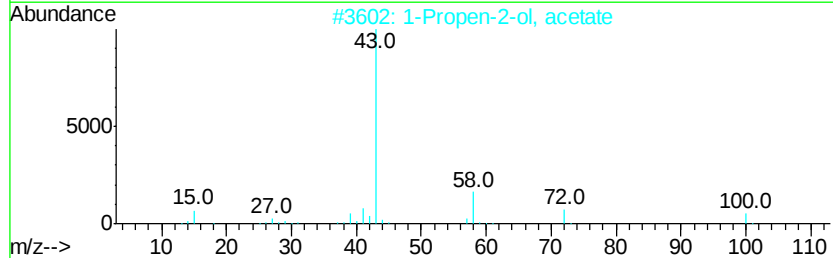
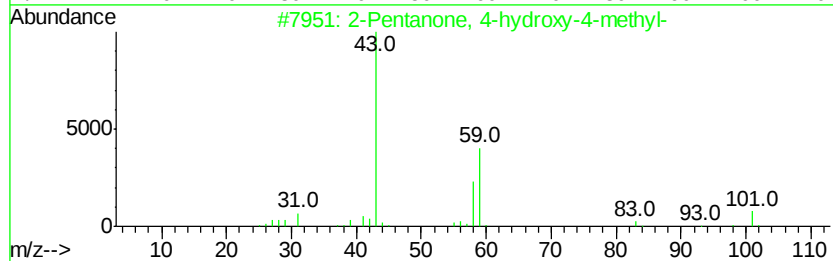
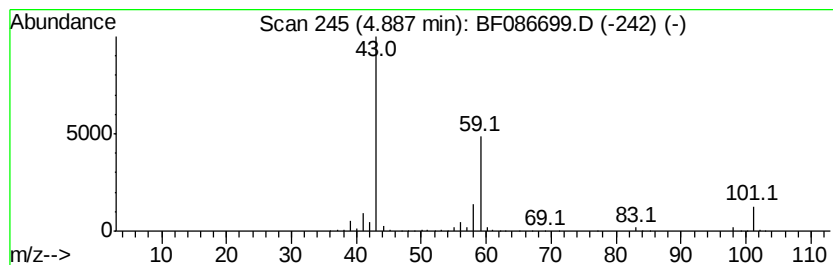
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	67.48 ng	1642910	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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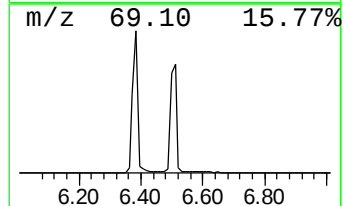
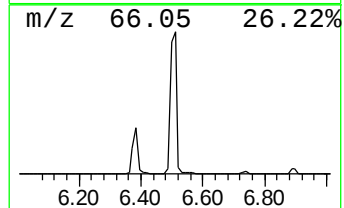
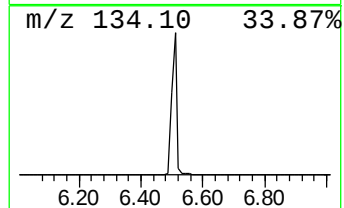
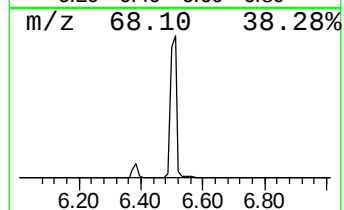
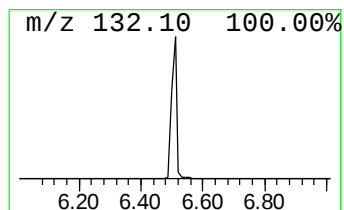
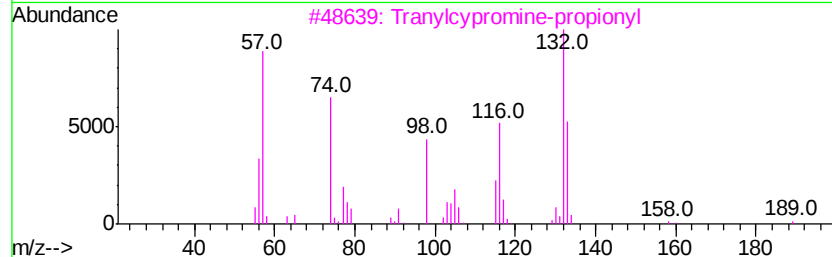
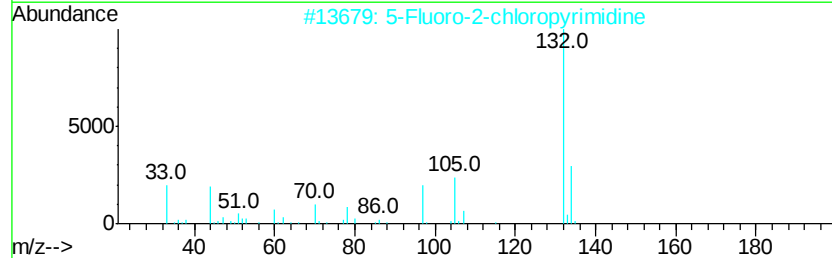
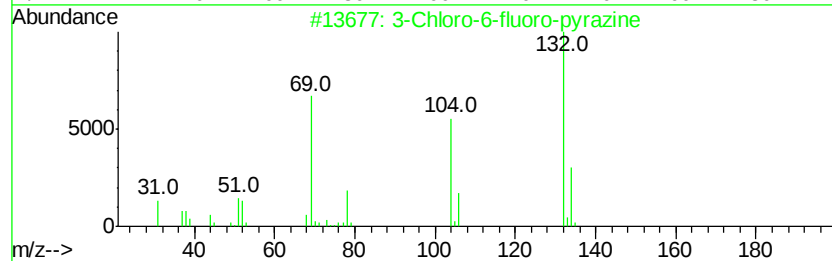
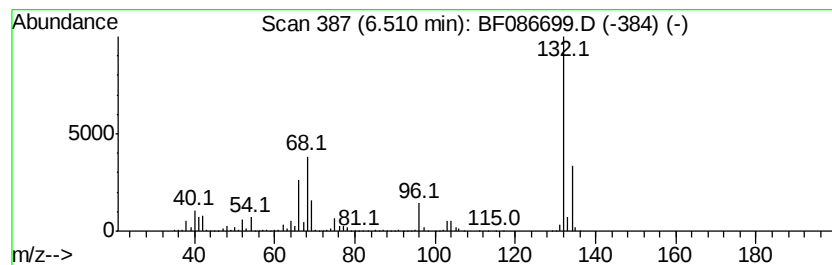
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	138.50 ng	3371910	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	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	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12		
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12		
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9		



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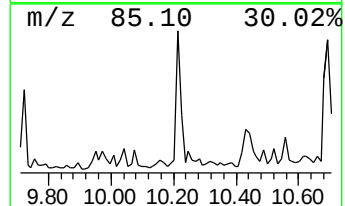
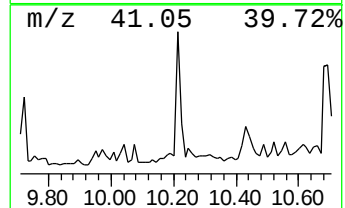
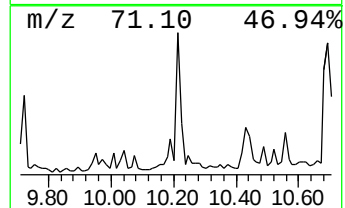
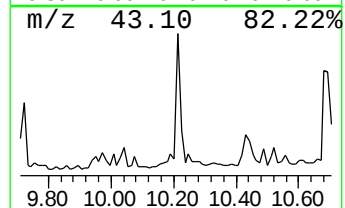
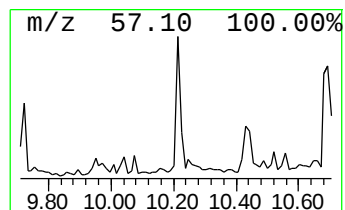
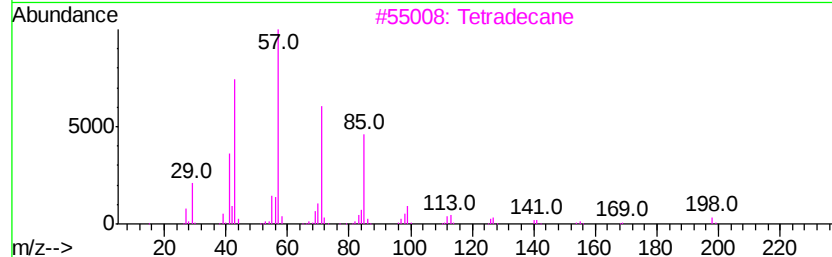
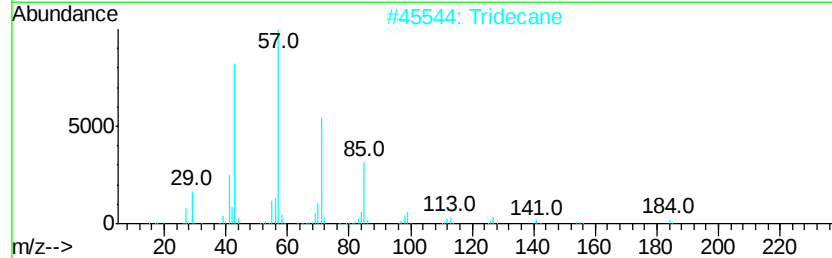
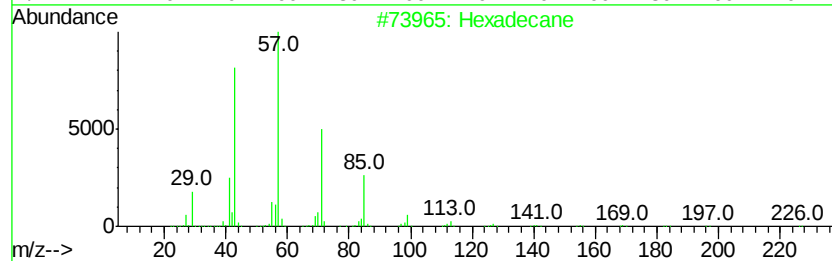
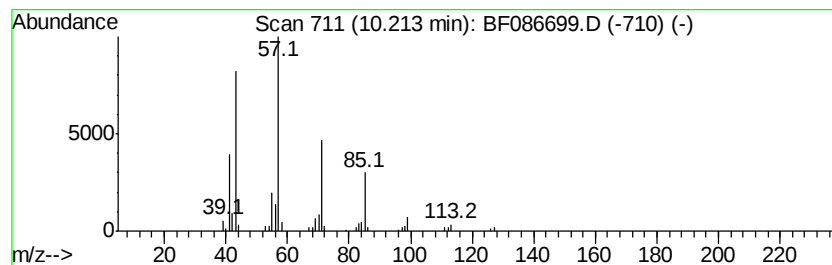
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	5.15 ng	128148	Acenaphthene-d10	9.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tridecane		184	C13H28	000629-50-5	86
3	Tetradecane		198	C14H30	000629-59-4	64
4	Heptadecane, 2,6-dimethyl-		268	C19H40	054105-67-8	64
5	Pentadecane		212	C15H32	000629-62-9	53



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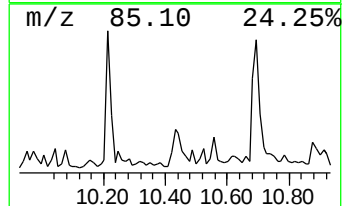
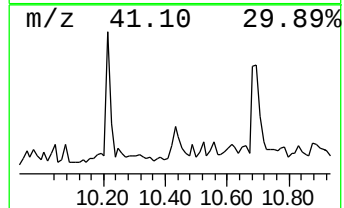
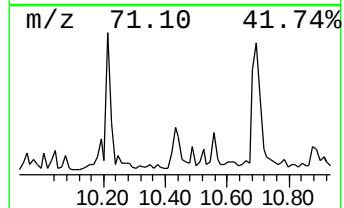
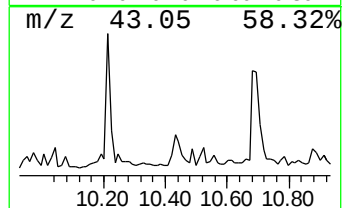
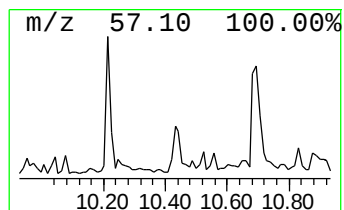
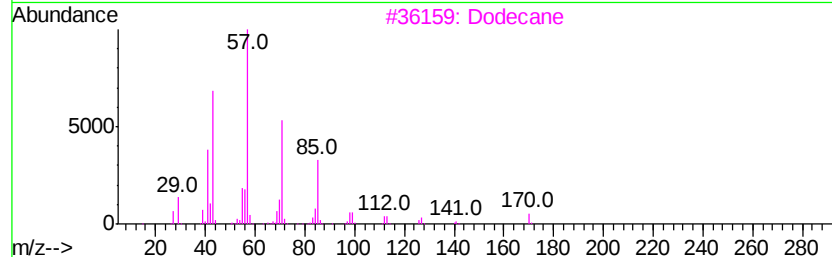
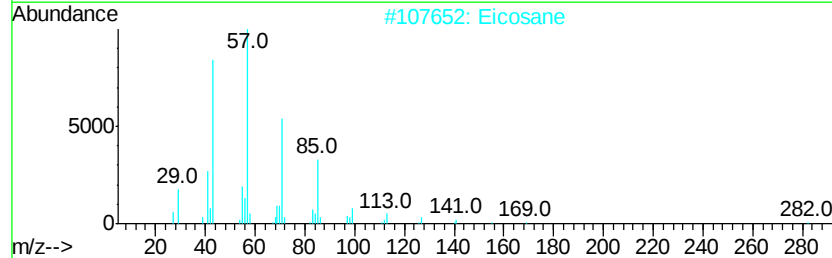
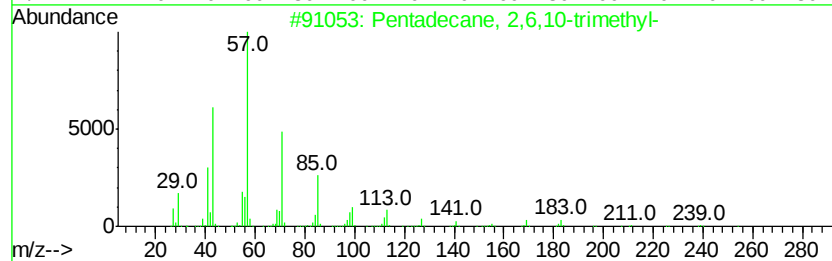
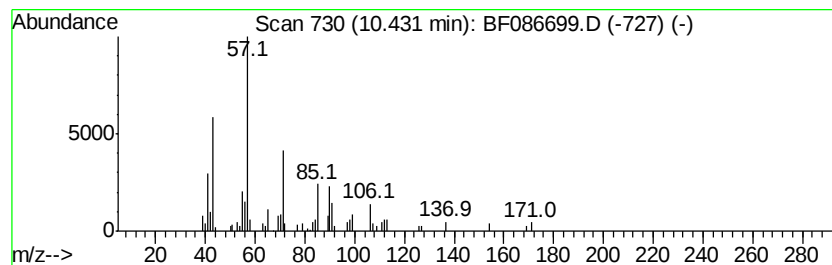
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	5.64 ng	140529	Acenaphthene-d10	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	52
2		Eicosane	282	C20H42	000112-95-8	52
3		Dodecane	170	C12H26	000112-40-3	52
4		Hexadecane	226	C16H34	000544-76-3	49
5		Tetracosane	338	C24H50	000646-31-1	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086699.D
Acq On : 5 May 2016 1:53
Operator : UM/SJ
Sample : H2715-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

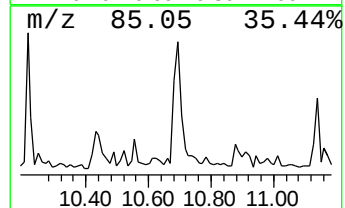
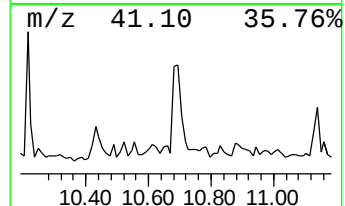
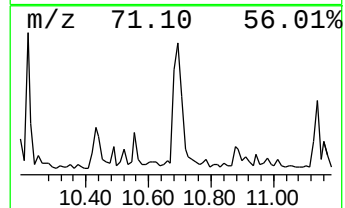
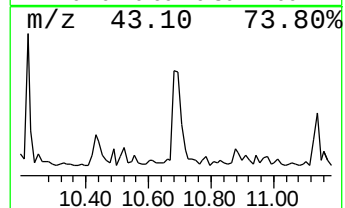
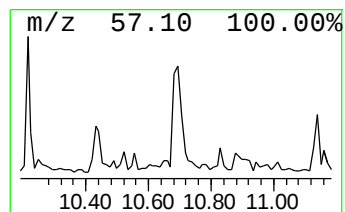
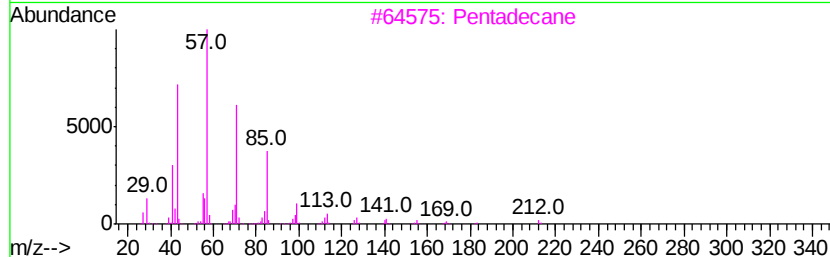
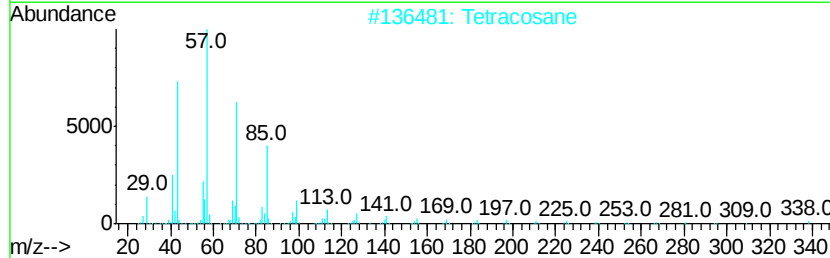
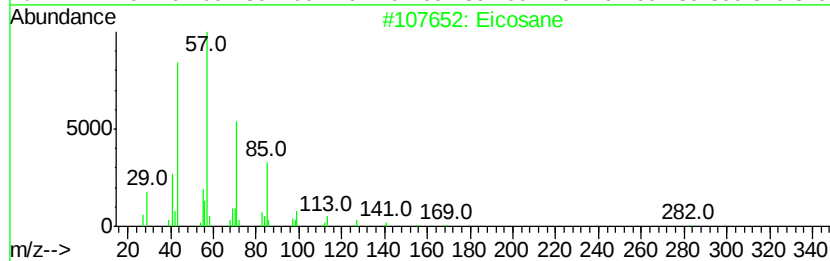
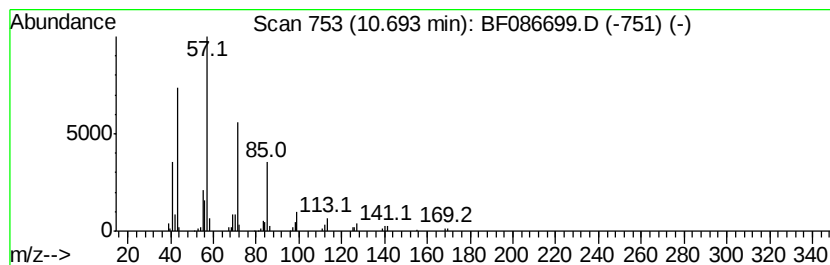
Instrument :
BNA_F
ClientSampleId :
26WARD-2-CS-3(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.69	9.01 ng	202577	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086699.D
Acq On : 5 May 2016 1:53
Operator : UM/SJ
Sample : H2715-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2-CS-3(0-10FTBGS)

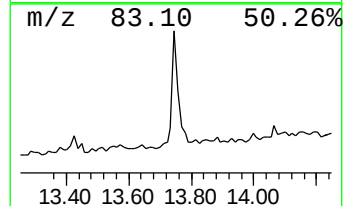
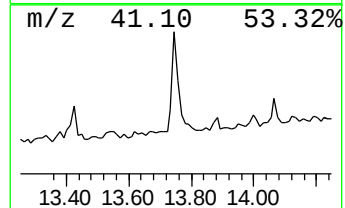
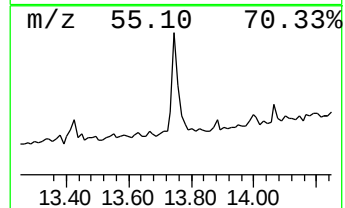
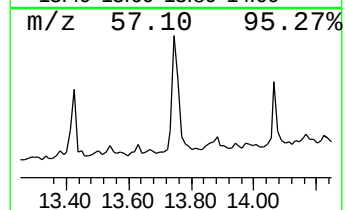
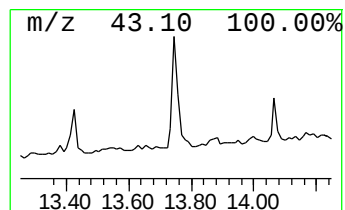
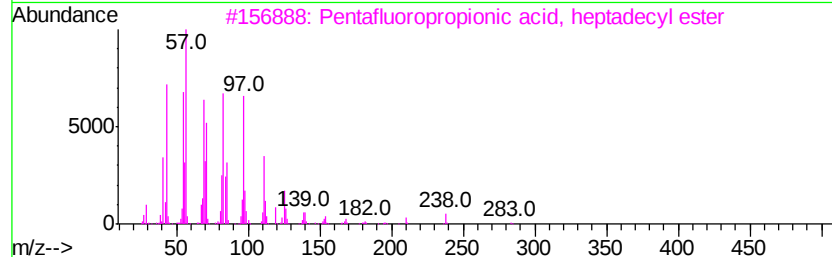
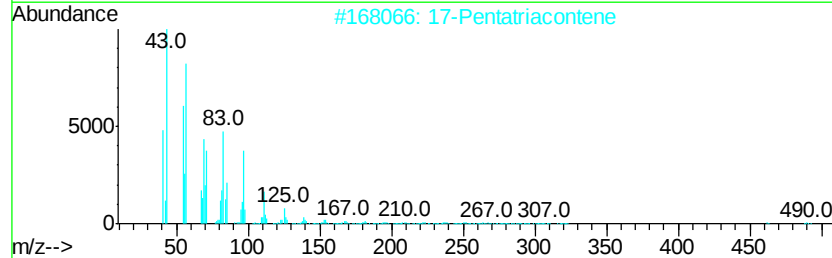
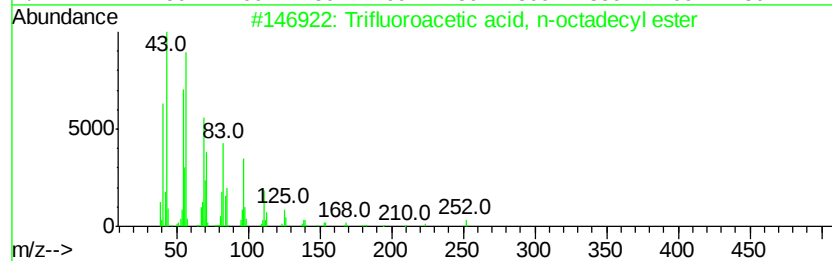
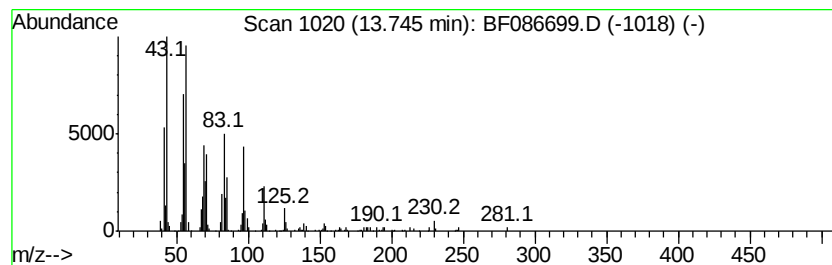
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetic acid, n-oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	6.91 ng	198474	Chrysene-d12	13.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	94
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086699.D
Acq On : 5 May 2016 1:53
Operator : UM/SJ
Sample : H2715-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2-CS-3(0-10FTBGS)

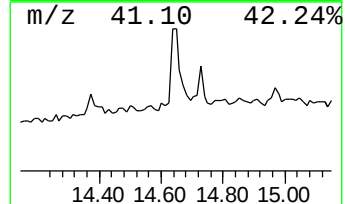
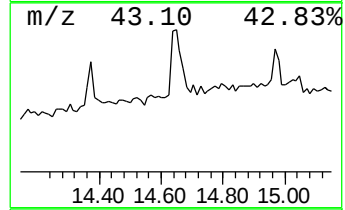
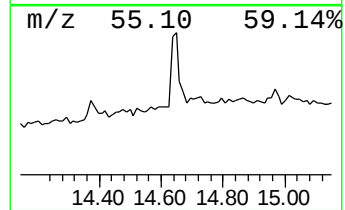
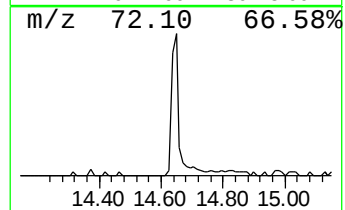
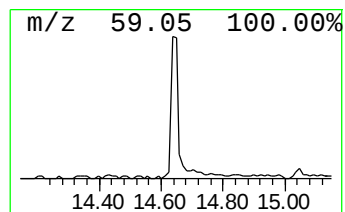
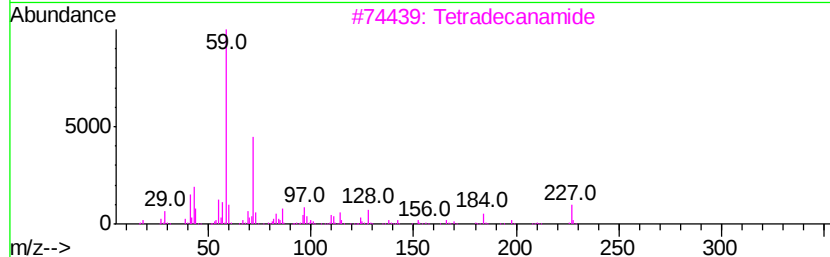
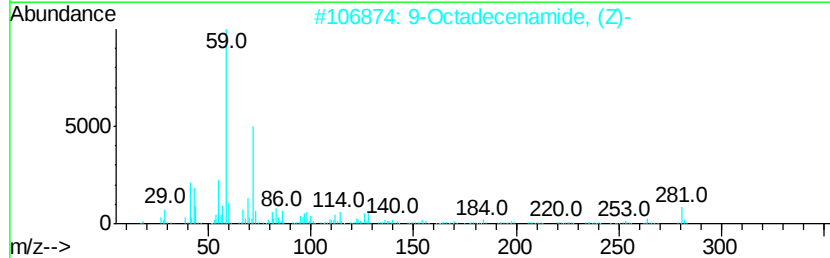
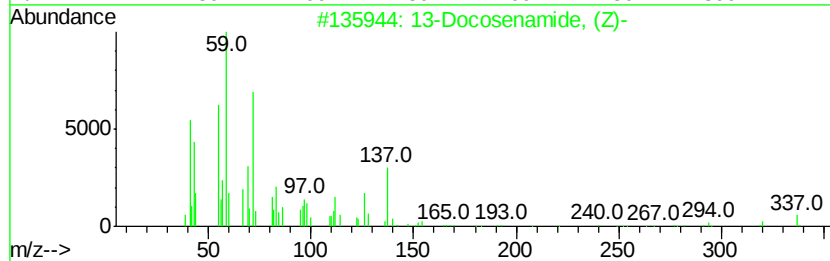
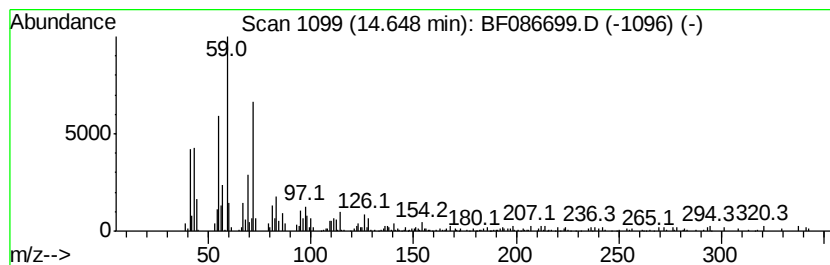
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	14.72 ng	264546	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3		Tetradecanamide	227	C14H29NO	000638-58-4	78
4		Hexadecanamide	255	C16H33NO	000629-54-9	53
5		2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086699.D
Acq On : 5 May 2016 1:53
Operator : UM/SJ
Sample : H2715-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2-CS-3(0-10FTBGS)

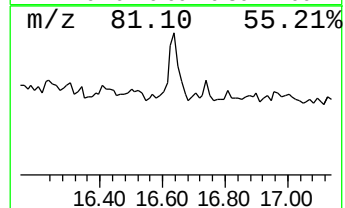
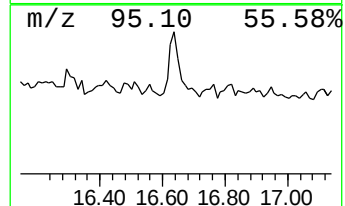
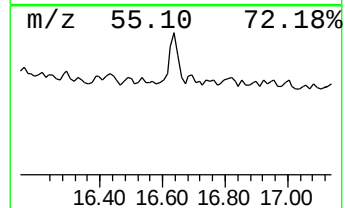
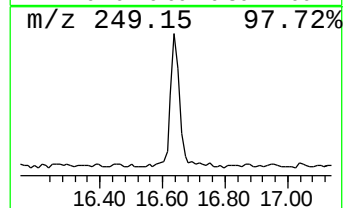
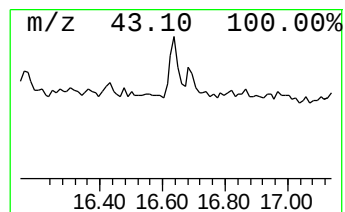
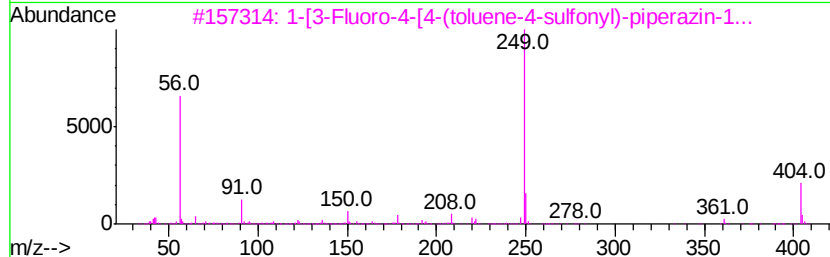
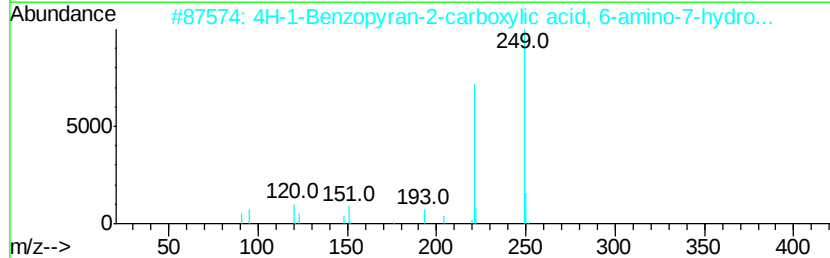
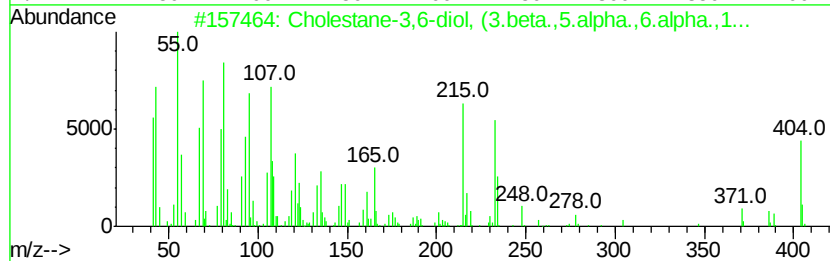
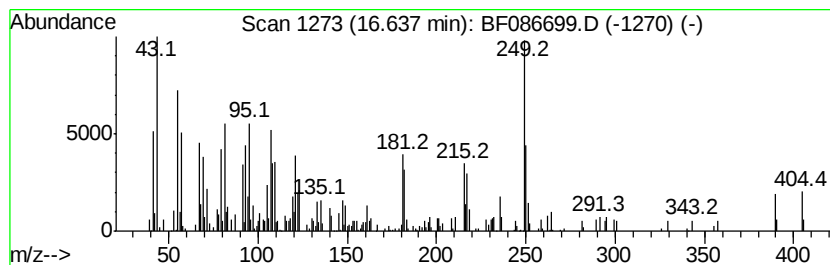
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.64 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	9.97 ng	179204	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	38
2		4H-1-Benzopyran-2-carboxylic aci...	249	C12H11NO5	030192-11-1	27
3		1-[3-Fluoro-4-[4-(toluene-4-sulf...	404	C21H25FN2O3S	333751-65-8	22
4		4H-1-Benzopyran-2-carboxylic aci...	249	C12H11NO5	030192-51-9	22
5		7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086699.D
Acq On : 5 May 2016 1:53
Operator : UM/SJ
Sample : H2715-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2-CS-3(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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-Penten-2-one, 4...	4.20	13.4	ng	325566	1	6.74	973825	40.0
2-Pentanone, 4-hy...	4.89	67.5	ng	1642910	1	6.74	973825	40.0
unknown6.51	6.51	138.5	ng	3371910	1	6.74	973825	40.0
Hexadecane	10.21	5.2	ng	128148	3	9.78	995787	40.0
Pentadecane, 2,6,...	10.43	5.6	ng	140529	3	9.78	995787	40.0
Eicosane	10.69	9.0	ng	202577	4	11.25	899598	40.0
Trifluoroacetic a...	13.75	6.9	ng	198474	5	13.88	1148460	40.0
13-Docosenamide, ...	14.65	14.7	ng	264546	6	15.28	718807	40.0
unknown16.64	16.64	10.0	ng	179204	6	15.28	718807	40.0