

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
 Data File : BF085725.D
 Acq On : 24 Mar 2016 20:40
 Operator : UM/SJ
 Sample : H1864-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-5

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-BF032416.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	4.996	235	237	247	rVB	79977	116722	3.21%	0.484%
2	5.419	272	274	276	rBV	995344	1189061	32.71%	4.935%
3	6.447	362	364	371	rVB	668133	747943	20.58%	3.104%
4	6.584	374	376	379	rBV	1871052	2131297	58.63%	8.845%
5	6.824	394	397	399	rBV	736609	662909	18.24%	2.751%
6	6.984	408	411	413	rBV	1712489	2290059	63.00%	9.504%
7	7.384	444	446	449	rBV	1305933	1893754	52.10%	7.859%
8	7.487	453	455	459	rVB	33178	50511	1.39%	0.210%
9	7.716	473	475	478	rBV3	50497	69757	1.92%	0.290%
10	7.853	483	487	490	rVV2	85239	111195	3.06%	0.461%
11	7.922	490	493	498	rVB3	35089	72105	1.98%	0.299%
12	8.105	507	509	512	rBV	878462	864815	23.79%	3.589%
13	8.470	539	541	544	rBV3	17754	45303	1.25%	0.188%
14	8.813	569	571	576	rVB	36507	49076	1.35%	0.204%
15	8.962	581	584	586	rBV3	23136	41176	1.13%	0.171%
16	9.190	601	604	606	rBV	3583066	3635078	100.00%	15.086%
17	9.305	609	614	615	rBV2	34948	59026	1.62%	0.245%
18	9.579	636	638	640	rBV	465912	378359	10.41%	1.570%
19	9.865	660	663	665	rBV	980316	1050652	28.90%	4.360%
20	10.002	671	675	676	rBV2	31795	48002	1.32%	0.199%
21	10.082	680	682	685	rBV2	60309	74354	2.05%	0.309%
22	10.288	696	700	702	rVB3	34123	80566	2.22%	0.334%
23	10.322	702	703	707	rBV4	19214	47611	1.31%	0.198%
24	10.653	729	732	734	rBV	1932556	2056313	56.57%	8.534%
25	10.768	741	742	746	rVB2	64232	95245	2.62%	0.395%
26	10.939	755	757	760	rBV4	23735	36743	1.01%	0.152%
27	11.019	762	764	767	rBV4	32500	49875	1.37%	0.207%
28	11.213	780	781	786	rVB2	48316	80574	2.22%	0.334%
29	11.339	790	792	795	rBV	934243	998721	27.47%	4.145%
30	11.579	810	813	816	rBV2	79986	113694	3.13%	0.472%
31	11.876	837	839	845	rBV2	292623	333216	9.17%	1.383%
32	12.596	899	902	905	rVB5	31726	57301	1.58%	0.238%
33	12.665	905	908	910	rBV	143540	202174	5.56%	0.839%
34	12.745	914	915	919	rVB3	102285	126197	3.47%	0.524%

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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

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35	12.814	919	921	928	rVB	130644	146193	4.02%	0.607%
36	12.928	928	931	934	rBV	2890688	2776513	76.38%	11.523%
37	13.819	1007	1009	1013	rBV	59387	108381	2.98%	0.450%
38	13.979	1020	1023	1025	rBV	487048	600128	16.51%	2.491%
39	15.397	1144	1147	1151	rBV	375840	532411	14.65%	2.210%
40	16.928	1278	1281	1293	rVB6	22685	72660	2.00%	0.302%

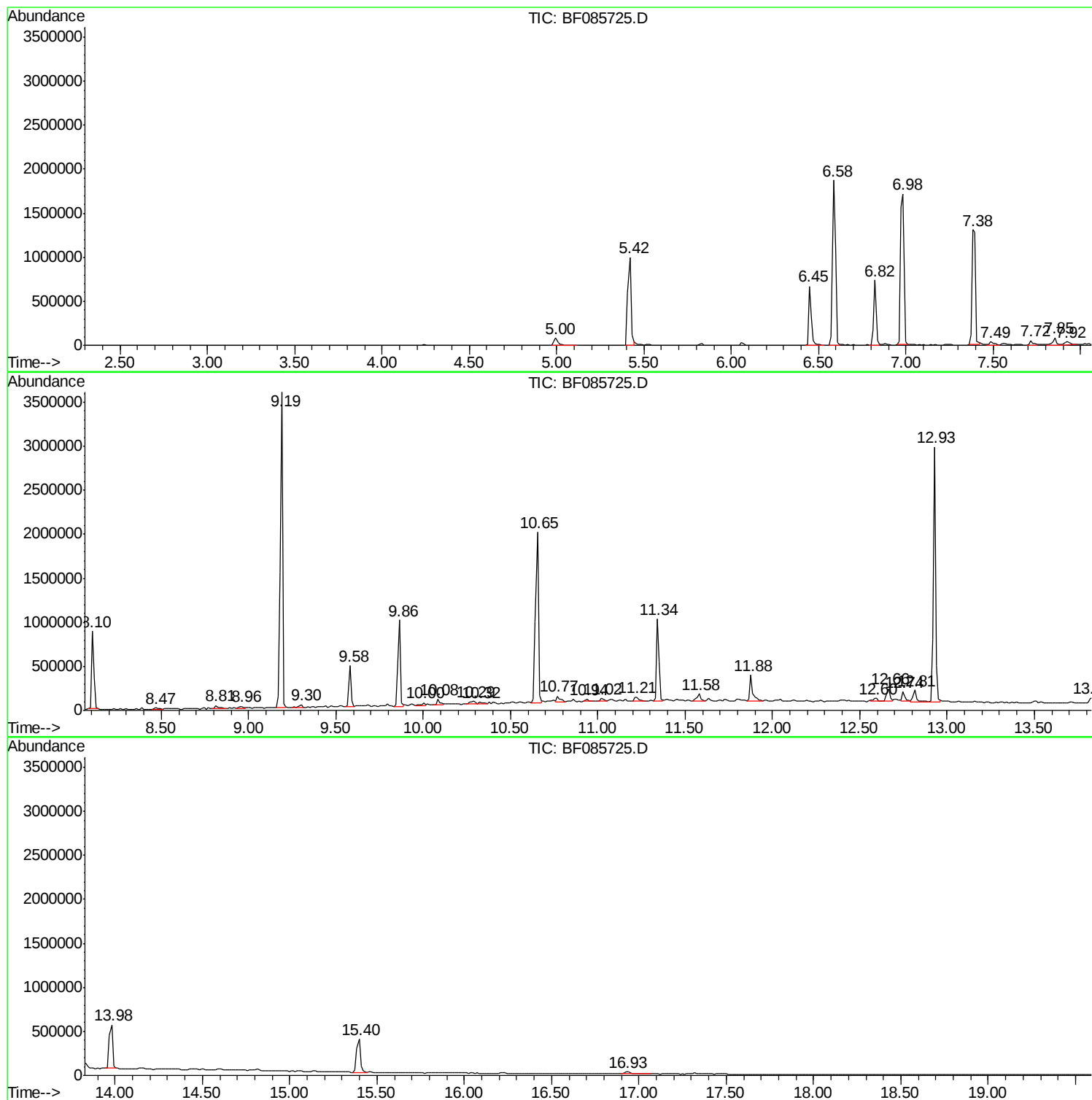
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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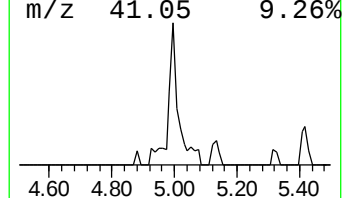
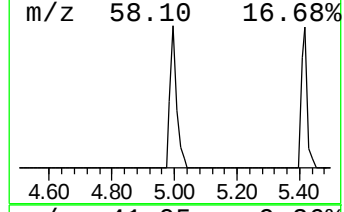
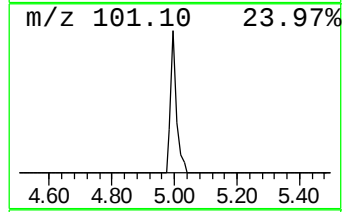
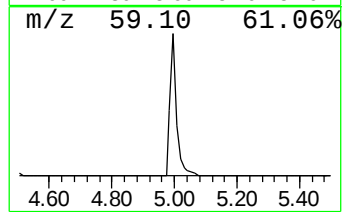
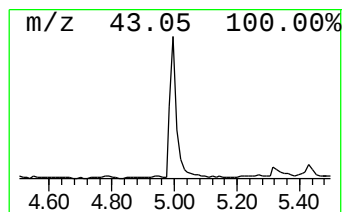
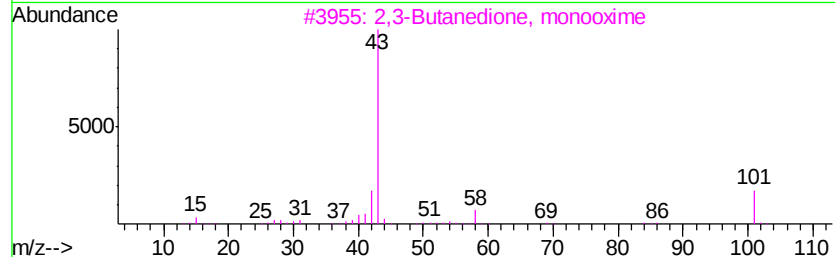
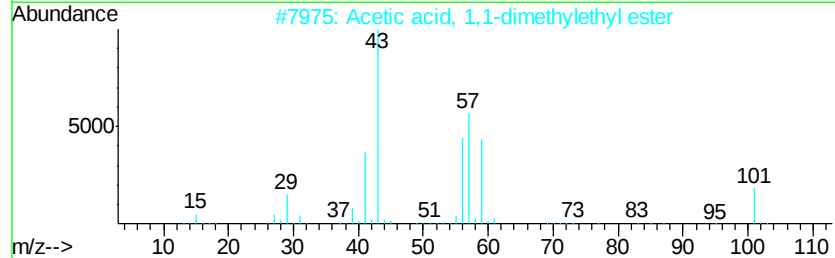
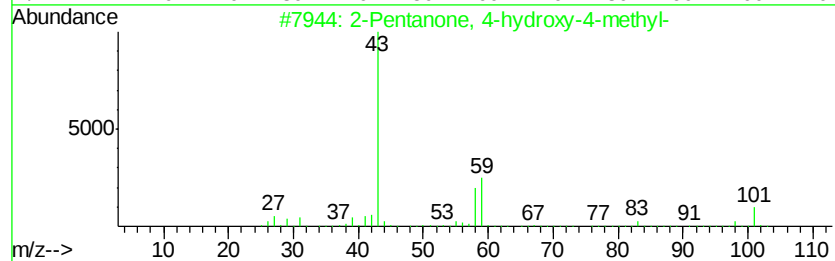
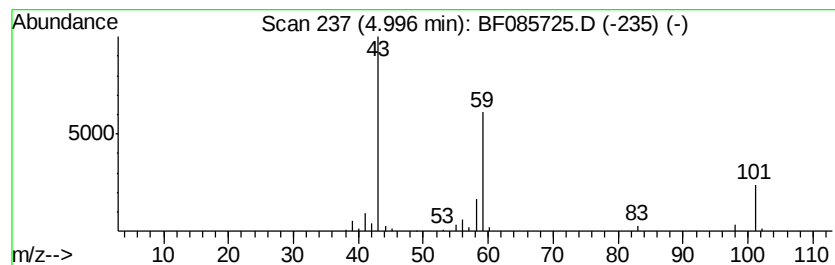
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.52 ng	116722	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol	102	C6H14O	000623-37-0	25
5			t-Butyl ethyl ether	102	C6H14O	1000118-18-4	17



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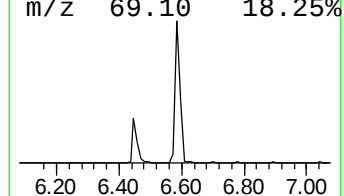
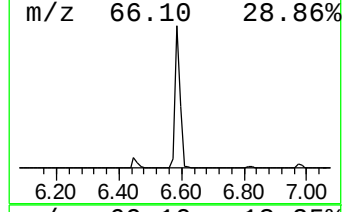
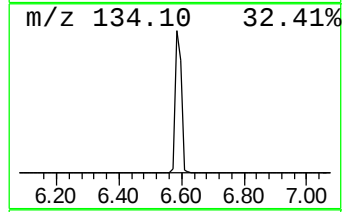
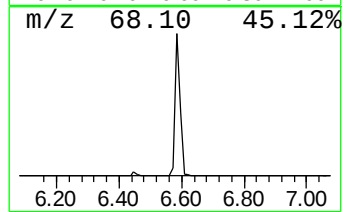
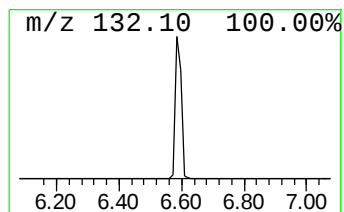
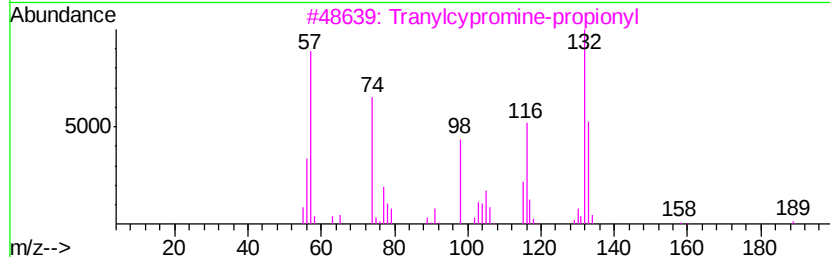
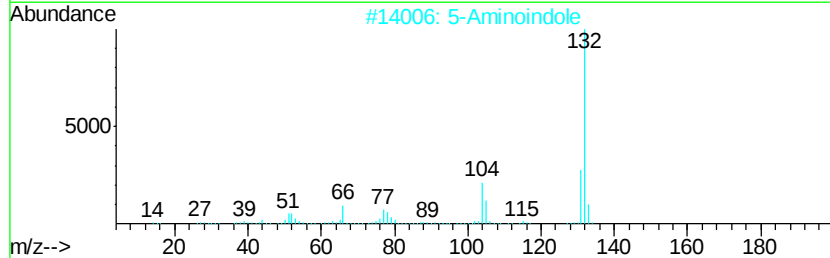
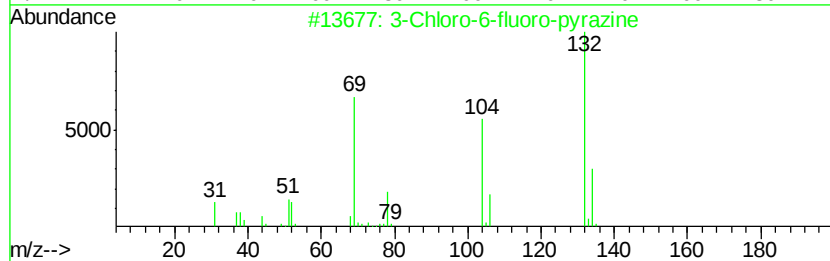
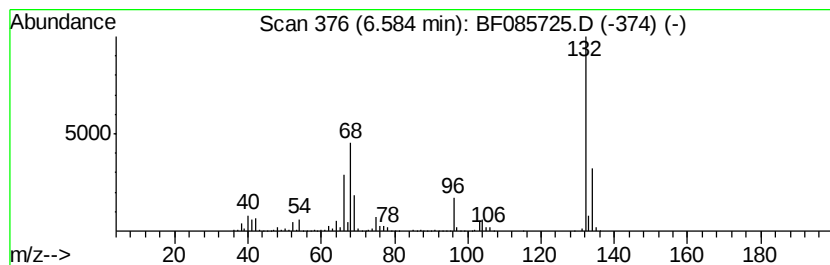
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	64.30 ng	2131300	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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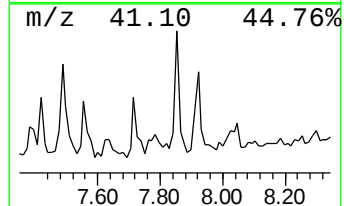
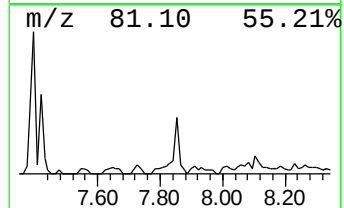
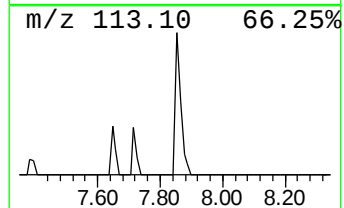
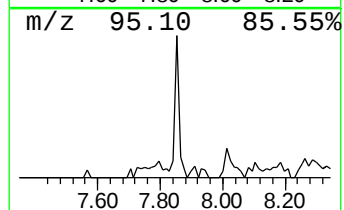
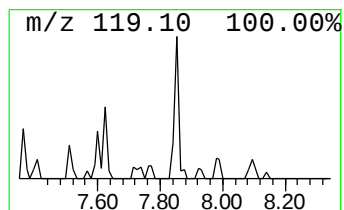
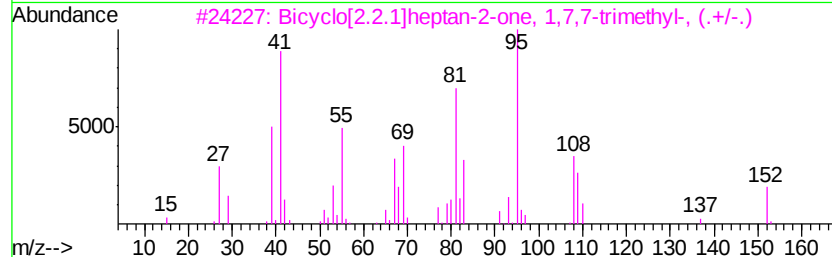
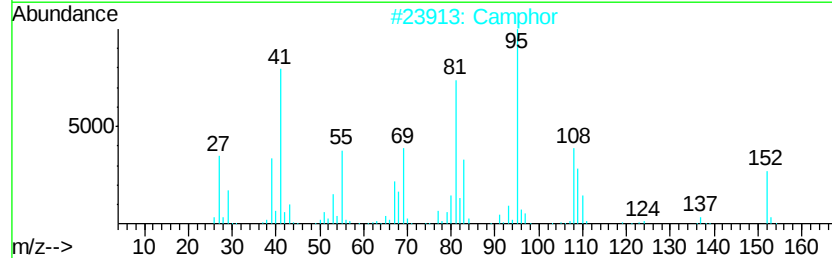
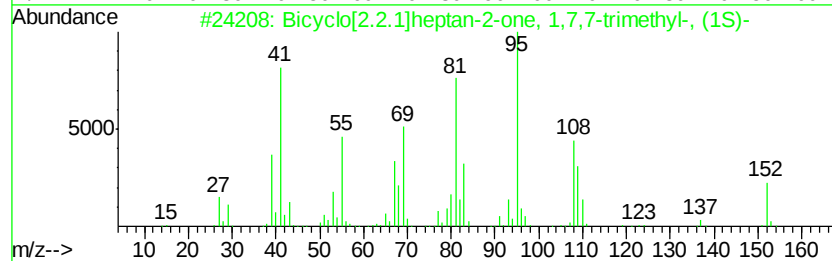
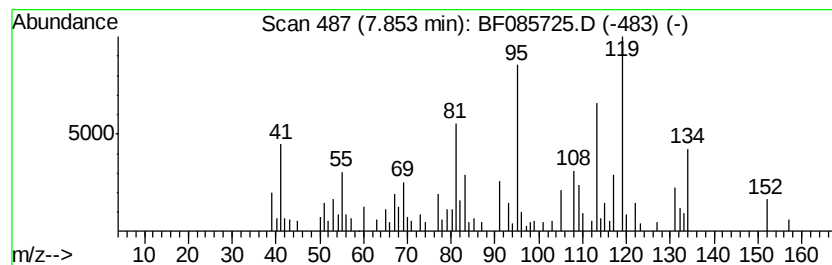
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.85	2.57 ng	111195	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	93
2		Camphor	152	C10H16O	000076-22-2	92
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	72
4		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	38
5		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	30



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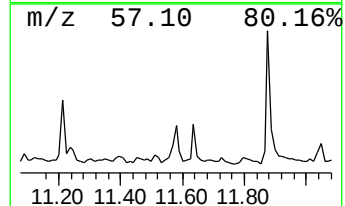
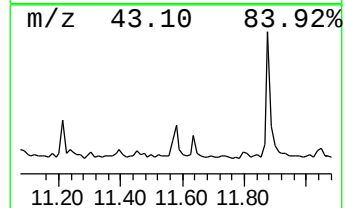
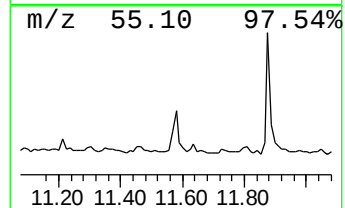
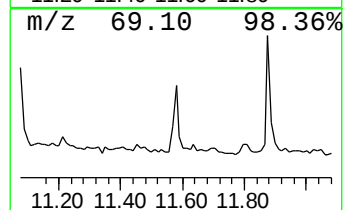
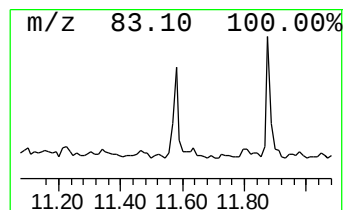
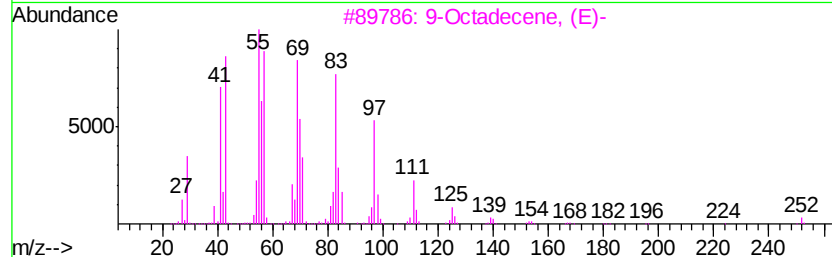
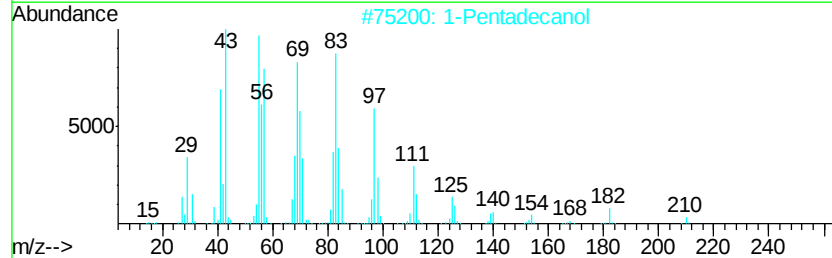
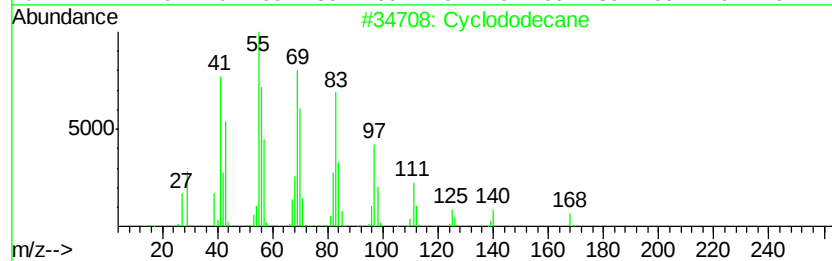
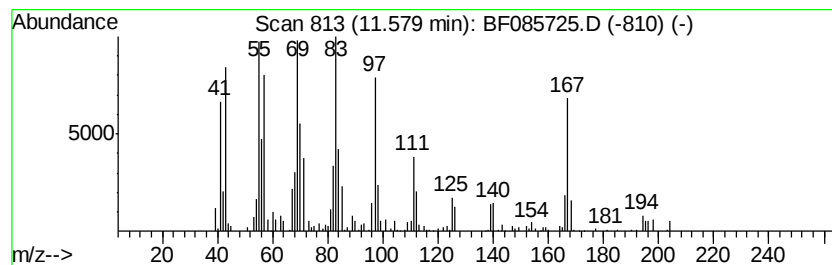
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Cyclododecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	2.28 ng	113694	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclododecane	168	C12H24	000294-62-2	94
2		1-Pentadecanol	228	C15H32O	000629-76-5	90
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	90
4		1-Tetradecanol	214	C14H30O	000112-72-1	90
5		1-Hexadecanol	242	C16H34O	036653-82-4	90



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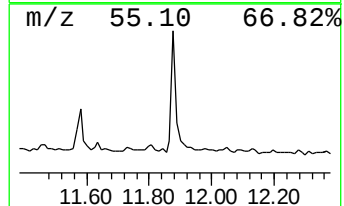
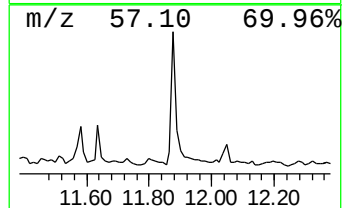
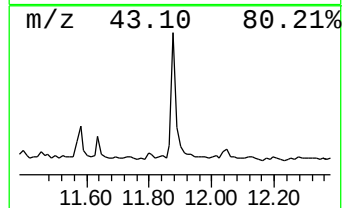
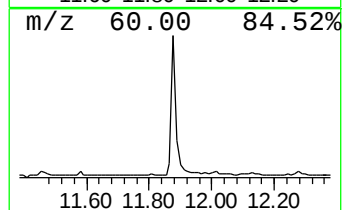
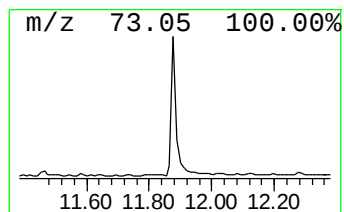
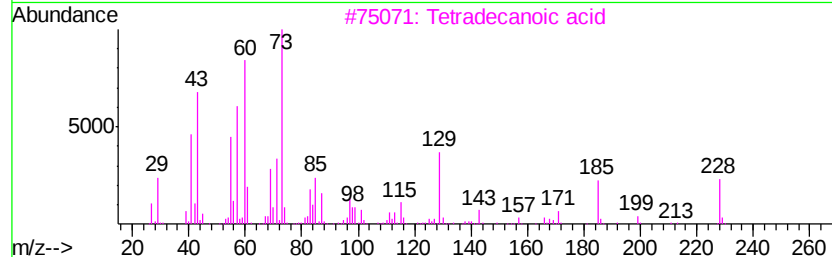
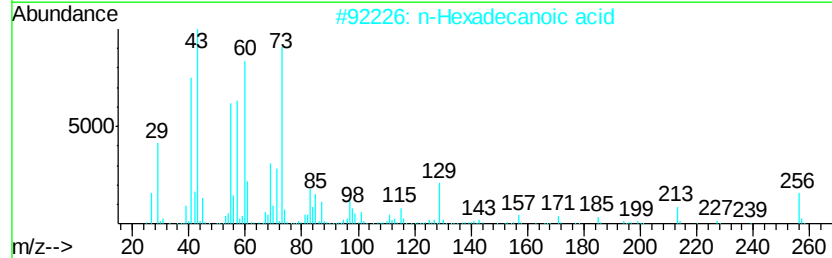
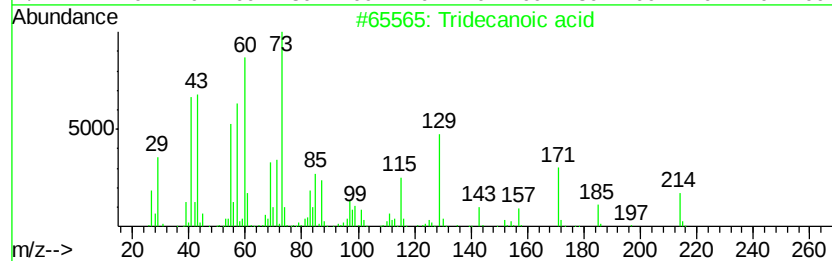
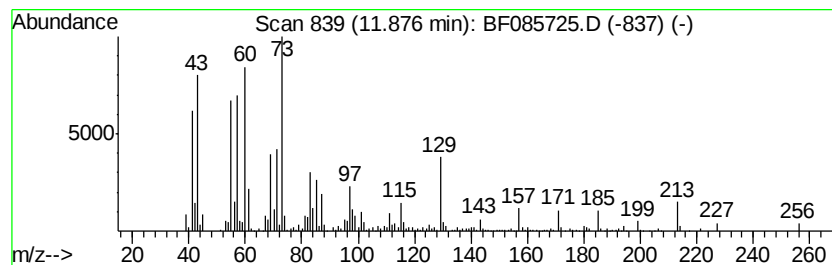
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Peak Number 6 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	6.67 ng	333216	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		n-Decanoic acid	172	C10H20O2	000334-48-5	81
5		Tridecane	184	C13H28	000629-50-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085725.D
Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

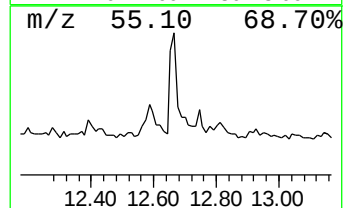
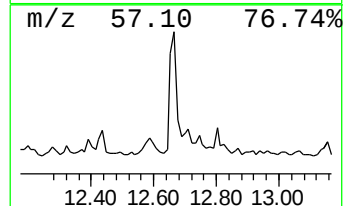
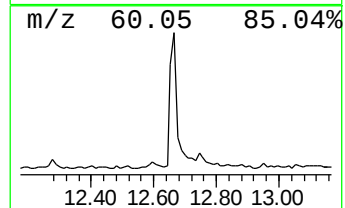
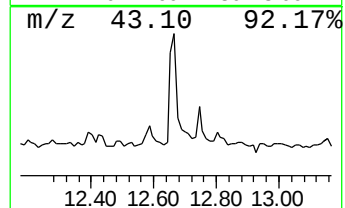
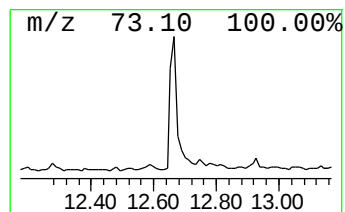
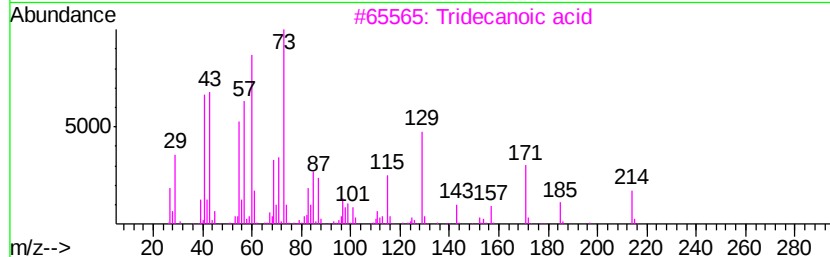
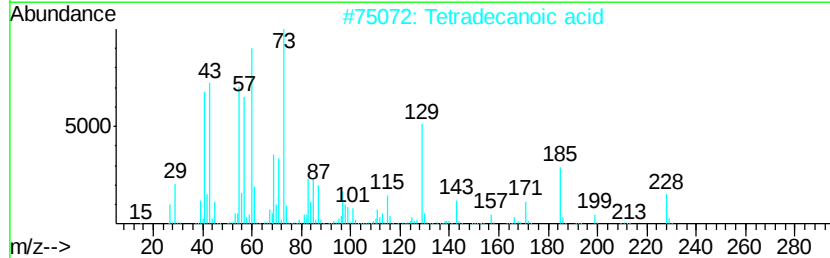
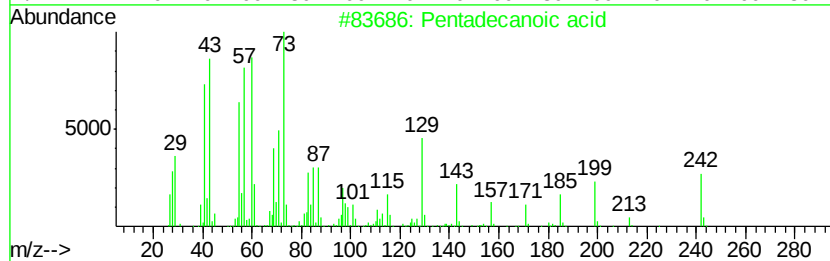
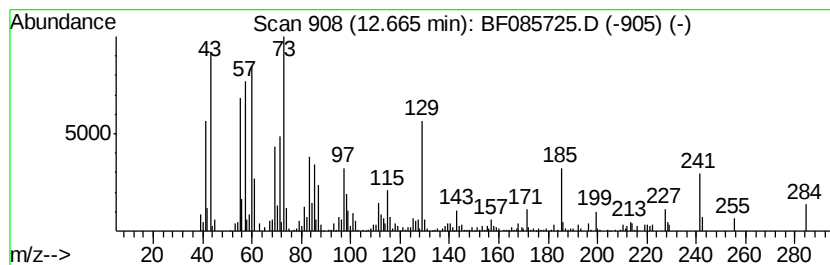
Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.67	6.74 ng	202174	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Undecanoic acid	186	C11H22O2	000112-37-8	52
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085725.D
Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

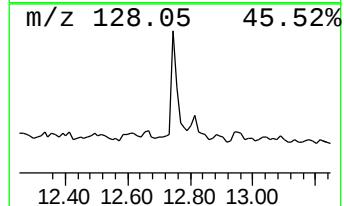
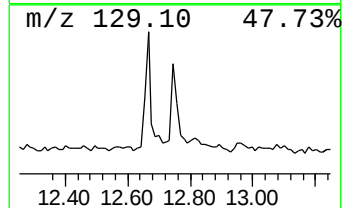
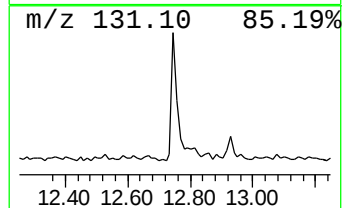
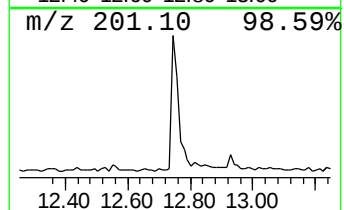
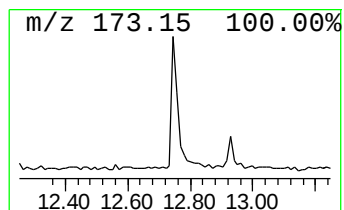
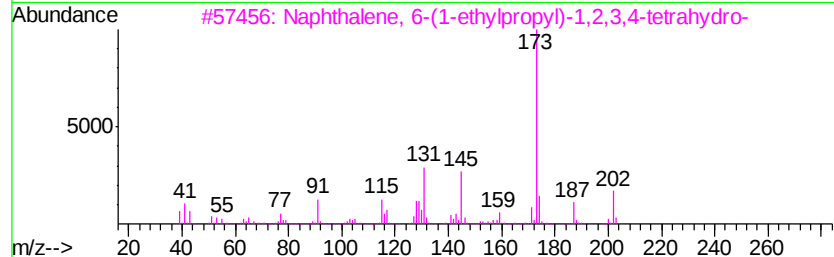
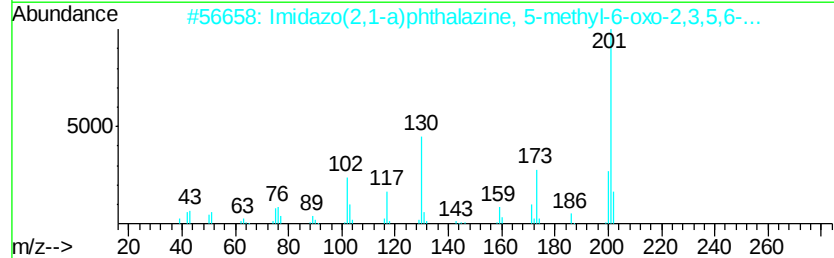
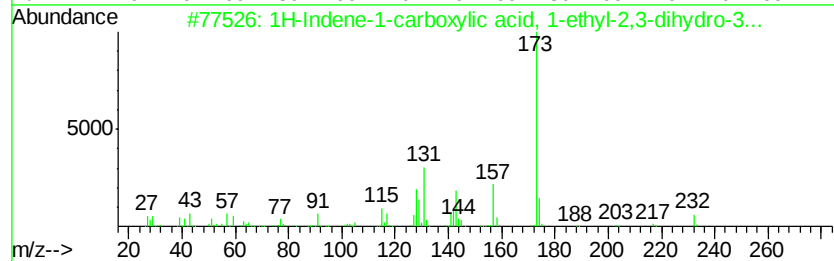
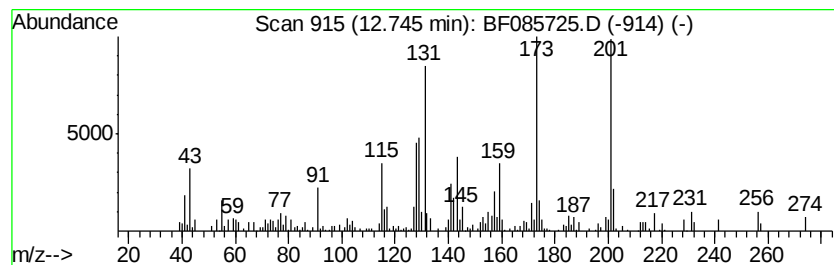
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown12.75 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	4.21 ng	126197	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene-1-carboxylic acid, 1-e...	232	C15H20O2	062185-65-3	25
2		Imidazo(2,1-a)phthalazine, 5-met...	201	C11H11N3O	057100-17-1	22
3		Naphthalene, 6-(1-ethylpropyl)-1...	202	C15H22	054889-56-4	22
4		7-Quinolinecarboxylic acid	173	C10H7NO2	001078-30-4	18
5		2,4-Quinolinedicarboxylic acid	217	C11H7NO4	005323-57-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085725.D
Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

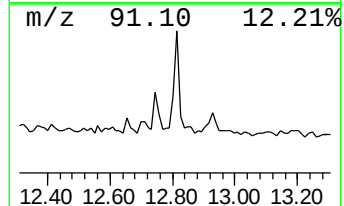
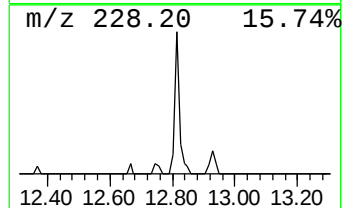
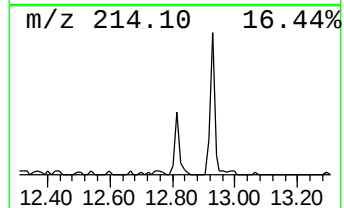
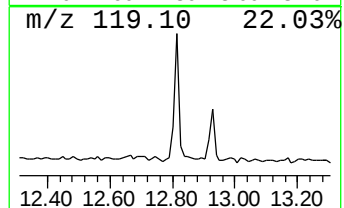
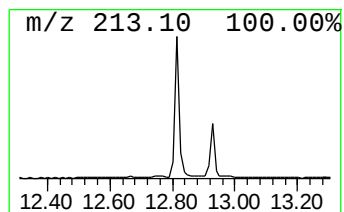
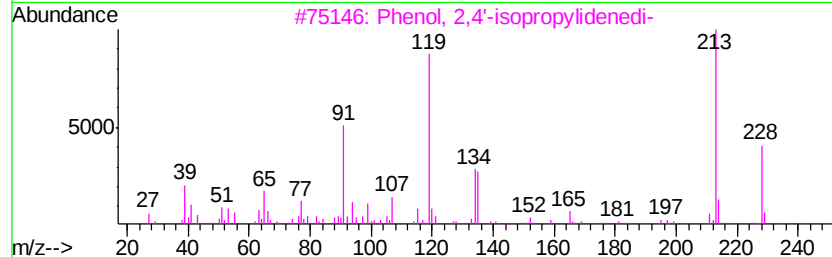
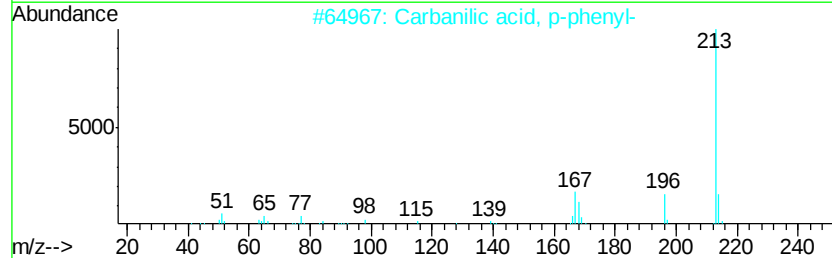
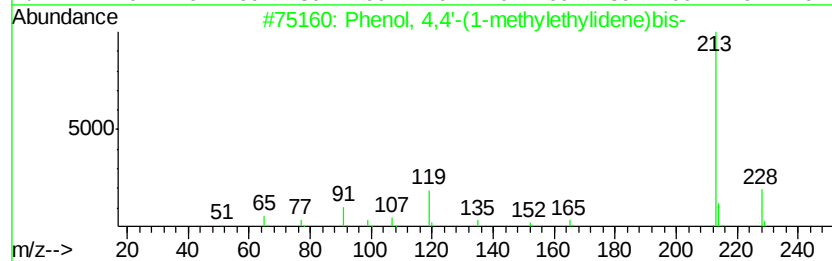
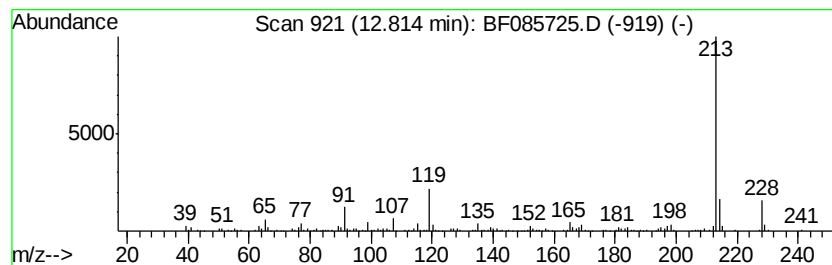
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	4.87 ng	146193	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96	
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	58	
3	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	56	
4	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	50	
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	42	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085725.D
Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

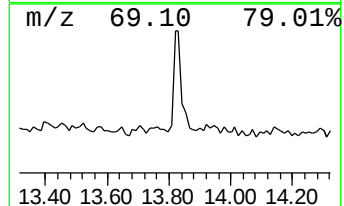
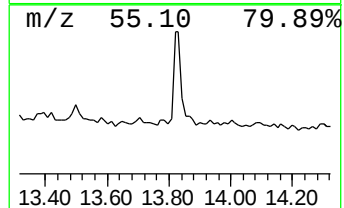
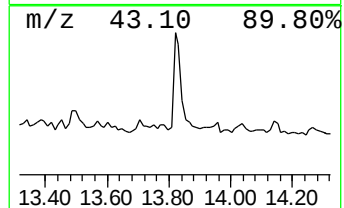
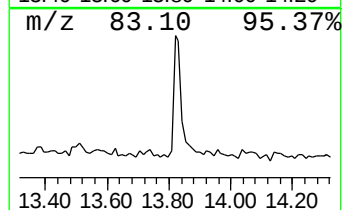
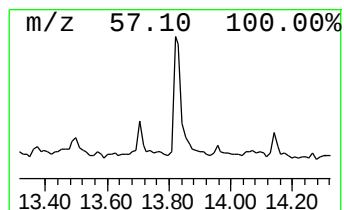
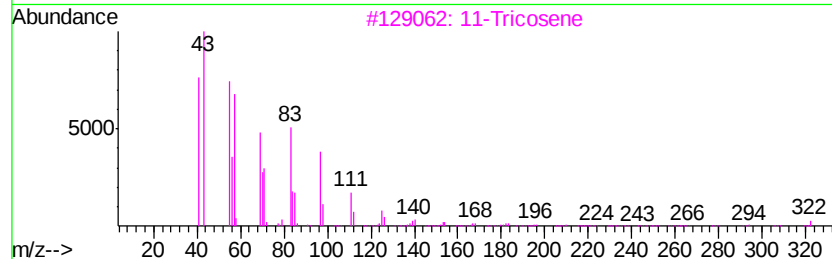
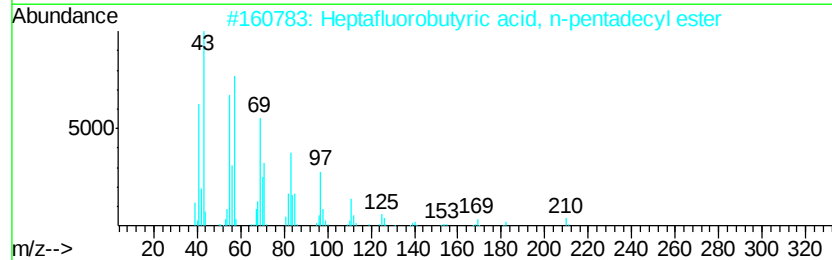
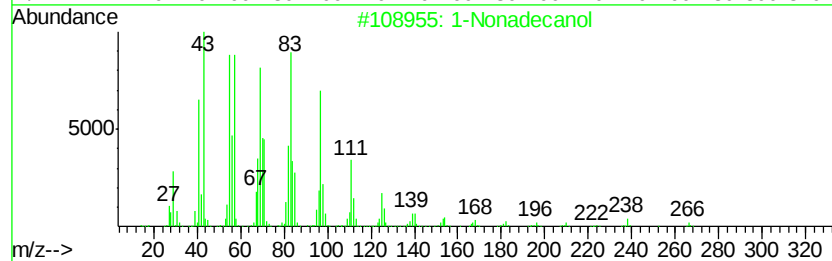
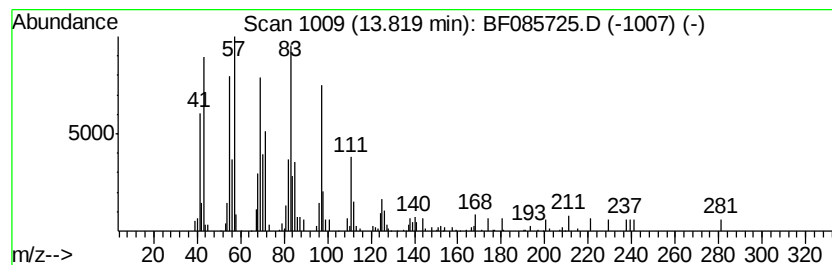
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	3.61 ng	108381	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecanol	284	C19H40O	001454-84-8	95
2	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085725.D
Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-5

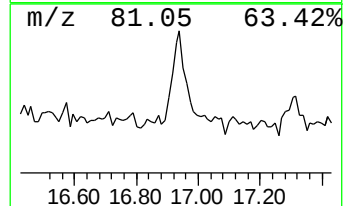
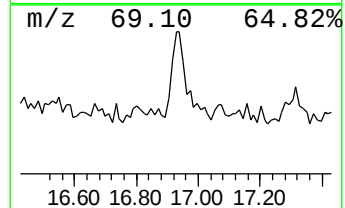
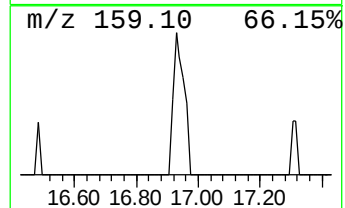
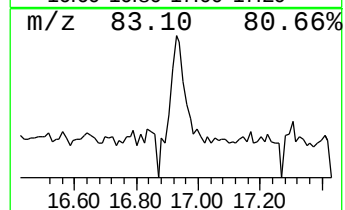
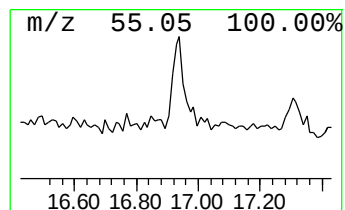
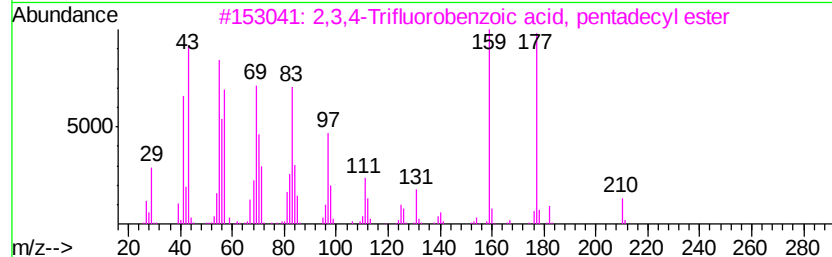
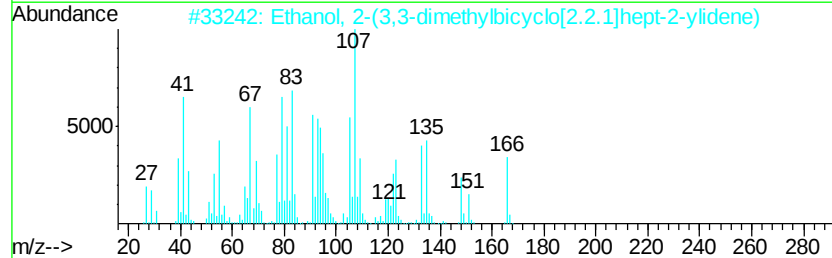
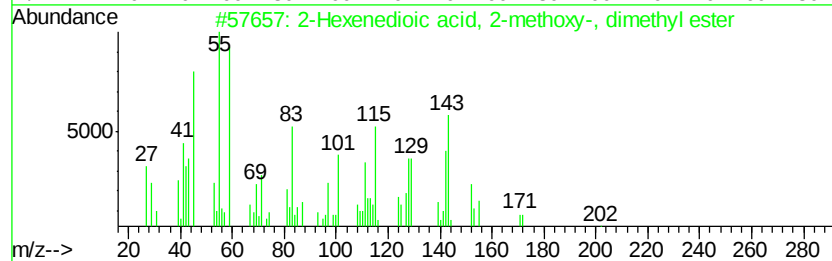
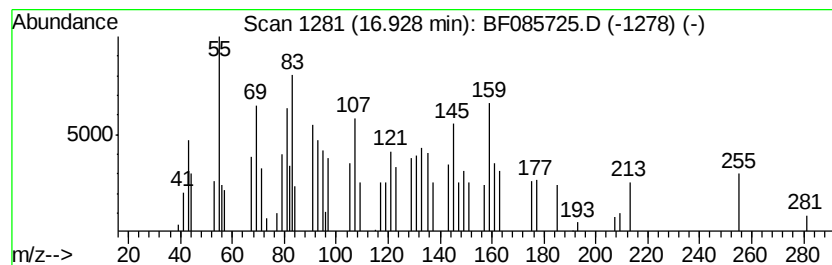
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	2.73 ng	72660	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexenedioic acid, 2-methoxy-, ...	202	C9H14O5	056114-71-7	22
2		Ethanol, 2-(3,3-dimethylbicyclo[...]	166	C11H18O	002226-05-3	14
3		2,3,4-Trifluorobenzoic acid, pen...	386	C22H33F3O2	1000280-45-4	12
4		2-Methyl-E,E-3,13-octadecadien-1-ol	280	C19H36O	1000130-90-6	12
5		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
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Acq On : 24 Mar 2016 20:40
Operator : UM/SJ
Sample : H1864-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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
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unknown6.58	6.58	64.3	ng	2131300	1	6.82	662909	20.0
Bicyclo[2.2.1]hep...	7.85	2.6	ng	111195	2	8.10	864815	20.0
Cyclododecane	11.58	2.3	ng	113694	4	11.34	998721	20.0
Tridecanoic acid	11.88	6.7	ng	333216	4	11.34	998721	20.0
Pentadecanoic acid	12.67	6.7	ng	202174	5	13.98	600128	20.0
unknown12.75	12.75	4.2	ng	126197	5	13.98	600128	20.0
Phenol, 4,4'-(1-m...	12.81	4.9	ng	146193	5	13.98	600128	20.0
1-Nonadecanol	13.82	3.6	ng	108381	5	13.98	600128	20.0
unknown16.93	16.93	2.7	ng	72660	6	15.40	532411	20.0