

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
 Data File : BF102839.D
 Acq On : 8 Feb 2018 2:37
 Operator : SJ/JU
 Sample : J1465-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3451

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-BF020318.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	2.163	9	13	26	rVB	341861	513509	13.48%	1.519%
2	5.110	511	514	522	rVB	167285	203623	5.35%	0.602%
3	5.504	576	581	584	rBV	3912082	3809372	100.00%	11.270%
4	6.510	747	752	755	rBV	3665107	3724845	97.78%	11.020%
5	6.651	772	776	780	rBV	3794244	3715164	97.53%	10.991%
6	6.886	812	816	819	rVB	1266893	1116519	29.31%	3.303%
7	7.039	838	842	846	rBV	3166845	2882291	75.66%	8.527%
8	7.445	906	911	914	rBV	2576799	2360163	61.96%	6.982%
9	8.169	1030	1034	1037	rBV	1535575	1395618	36.64%	4.129%
10	9.239	1212	1216	1219	rBV	3902163	3545399	93.07%	10.489%
11	9.316	1226	1229	1231	rVB	73561	54025	1.42%	0.160%
12	9.627	1279	1282	1285	rBV	182050	183837	4.83%	0.544%
13	9.845	1312	1319	1322	rBV	180203	147745	3.88%	0.437%
14	9.922	1328	1332	1340	rBV2	1443911	1292492	33.93%	3.824%
15	10.345	1401	1404	1407	rVB	184023	139698	3.67%	0.413%
16	10.563	1436	1441	1444	rBV	42802	56756	1.49%	0.168%
17	10.710	1462	1466	1478	rVB	1789638	1681371	44.14%	4.974%
18	10.816	1482	1484	1494	rVB	129205	139973	3.67%	0.414%
19	11.269	1558	1561	1563	rBV	61218	52478	1.38%	0.155%
20	11.410	1581	1585	1588	rBV	1267217	1055017	27.70%	3.121%
21	11.921	1665	1672	1678	rBV5	44401	66445	1.74%	0.197%
22	12.621	1788	1791	1795	rBV	73792	63254	1.66%	0.187%
23	12.851	1825	1830	1833	rBV	63181	68067	1.79%	0.201%
24	12.992	1850	1854	1858	rBV	2666718	2586038	67.89%	7.651%
25	13.451	1929	1932	1939	rVB3	187273	231010	6.06%	0.683%
26	13.880	2001	2005	2014	rBV	394581	430422	11.30%	1.273%
27	14.021	2025	2029	2030	rBV	62533	55482	1.46%	0.164%
28	14.051	2030	2034	2037	rVV	1097899	972514	25.53%	2.877%
29	14.510	2109	2112	2117	rBV2	43924	53927	1.42%	0.160%
30	14.815	2161	2164	2169	rVB	47275	55820	1.47%	0.165%
31	14.968	2187	2190	2196	rVB6	38166	41629	1.09%	0.123%
32	15.162	2219	2223	2226	rBV	70854	91130	2.39%	0.270%
33	15.533	2280	2286	2296	rBV	566882	853649	22.41%	2.525%
34	15.992	2360	2364	2368	rVB	70043	96114	2.52%	0.284%

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ClientSampleId :
RT-3451

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

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35	16.509	2449	2452	2458	rVB3	40975	65979	1.73%	0.195%
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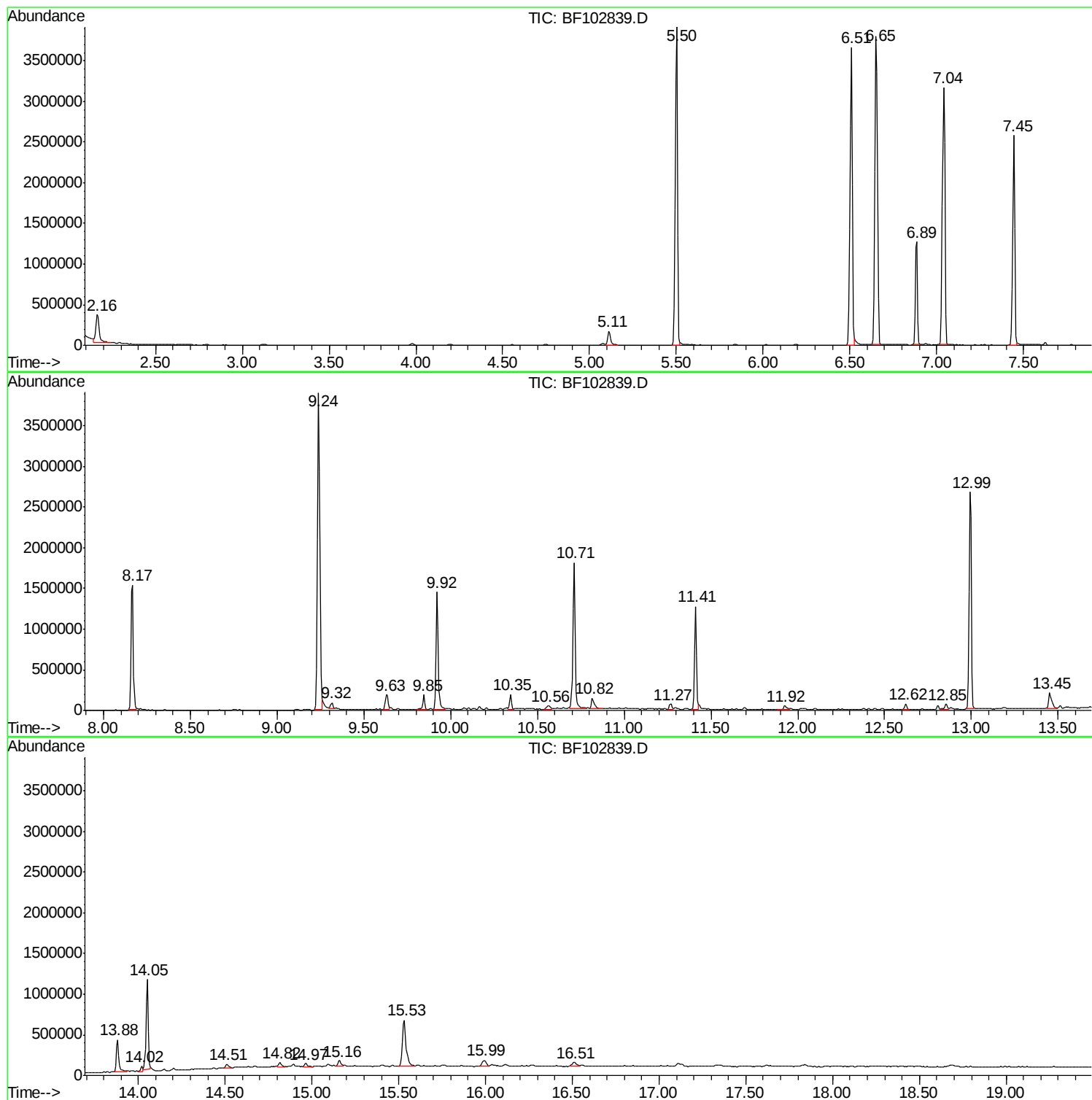
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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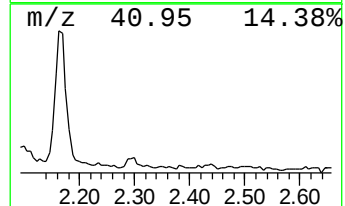
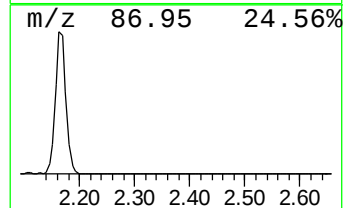
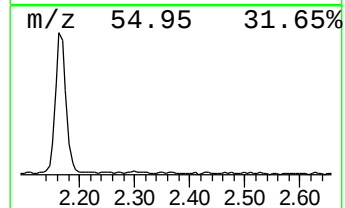
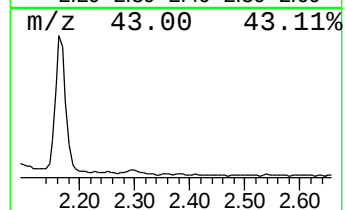
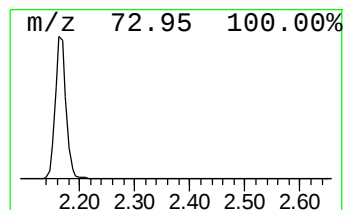
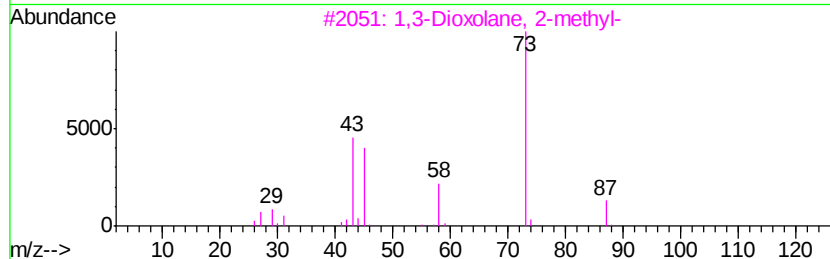
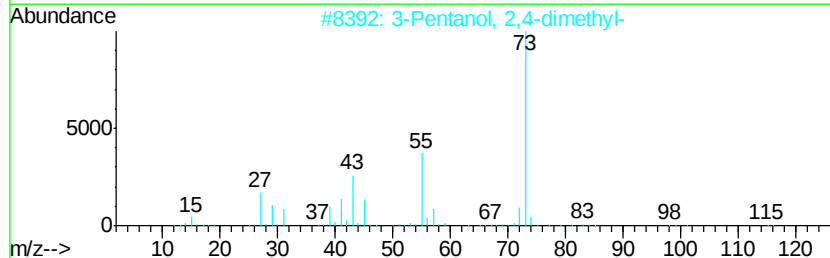
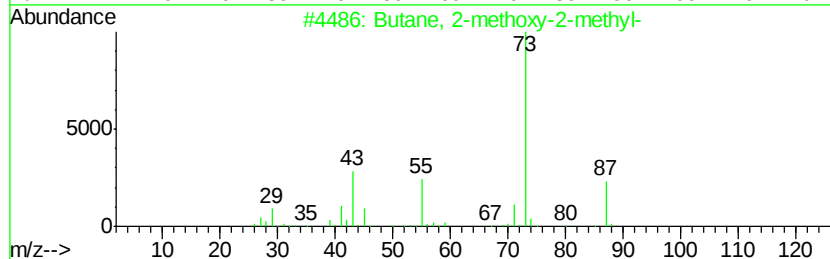
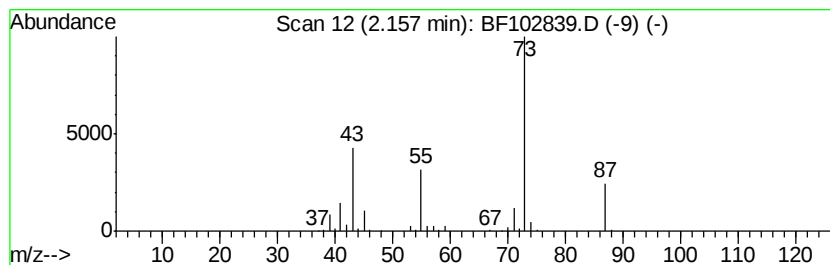
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.20 ng	513509	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	28



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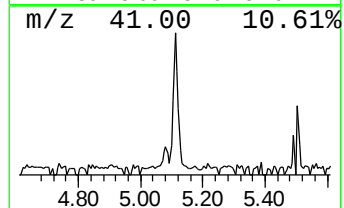
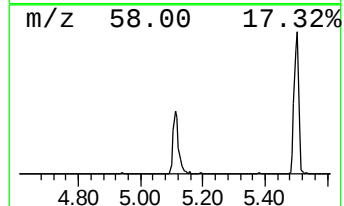
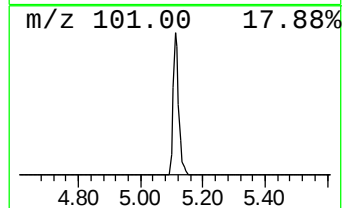
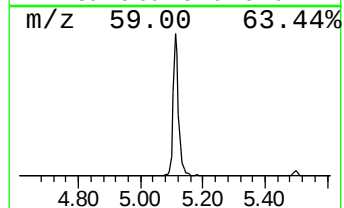
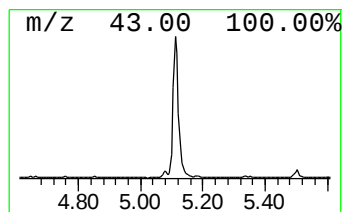
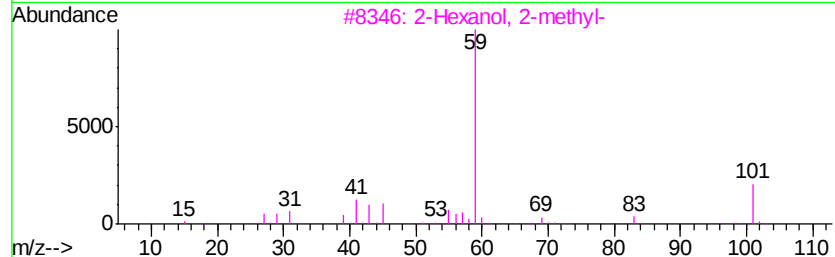
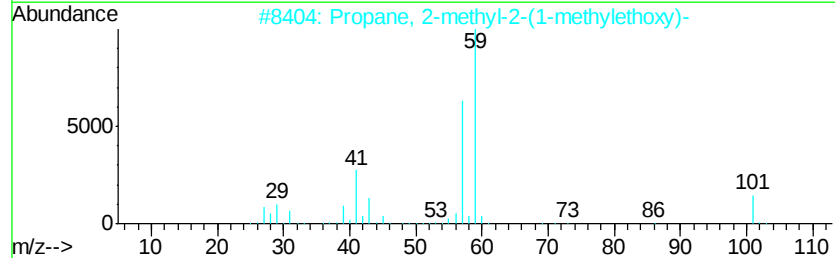
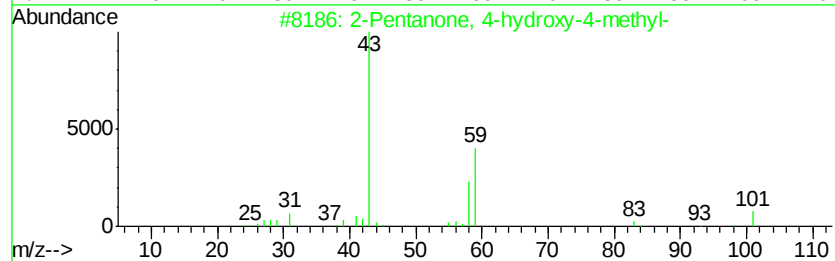
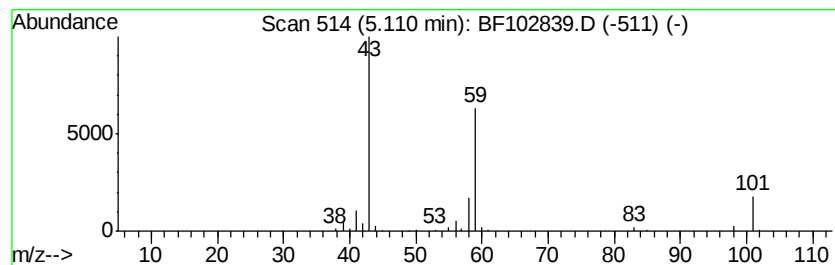
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.65 ng	203623	1,4-Dichlorobenzene-d4	6.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Acetone	58	C3H6O	000067-64-1	9	



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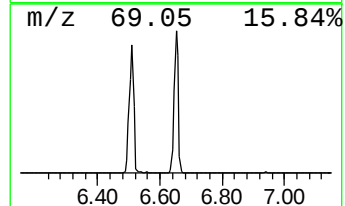
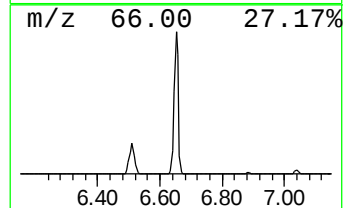
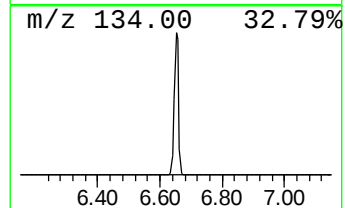
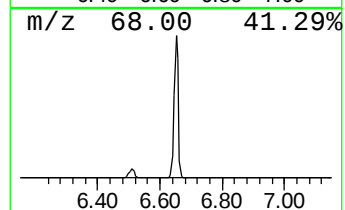
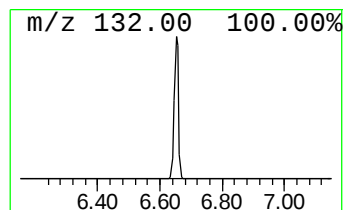
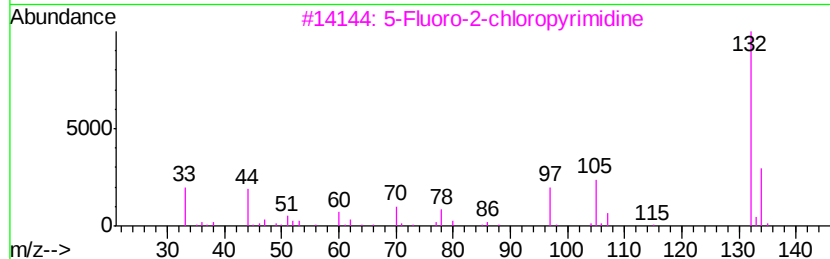
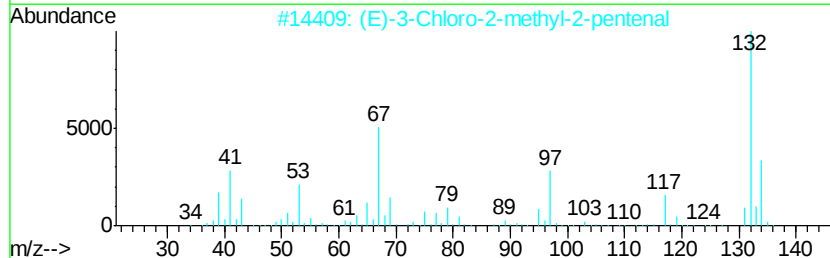
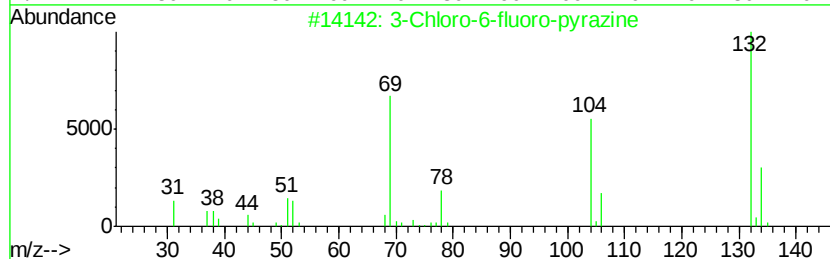
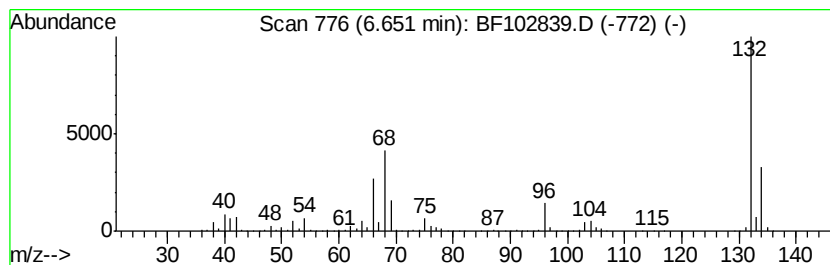
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.55 ng	3715160	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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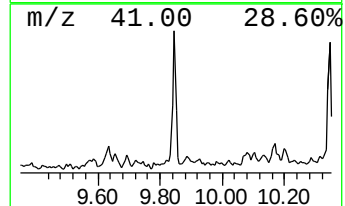
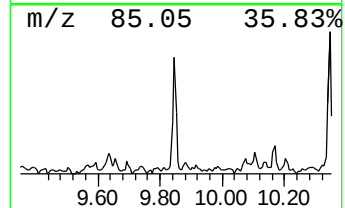
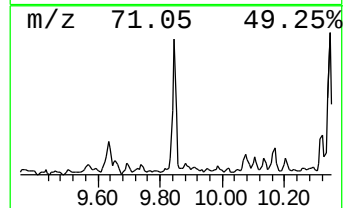
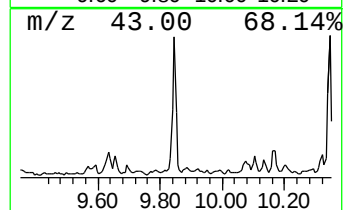
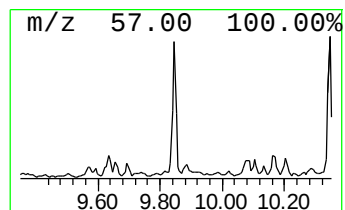
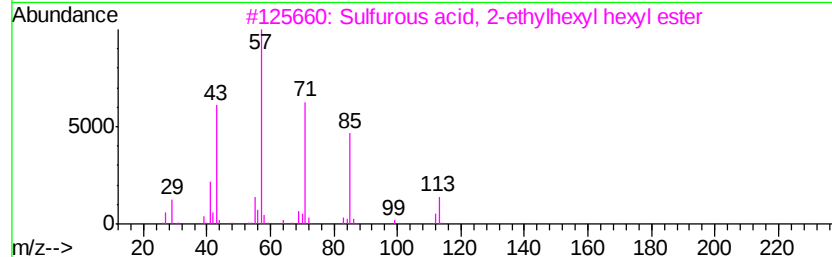
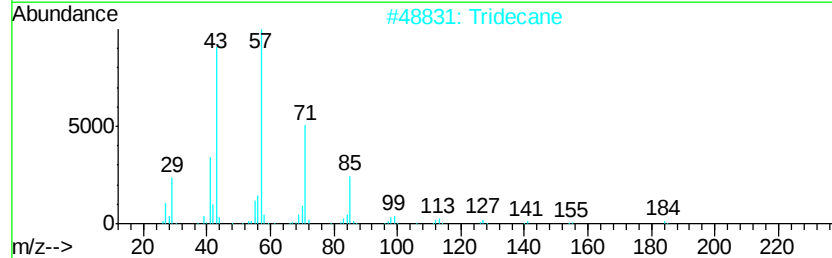
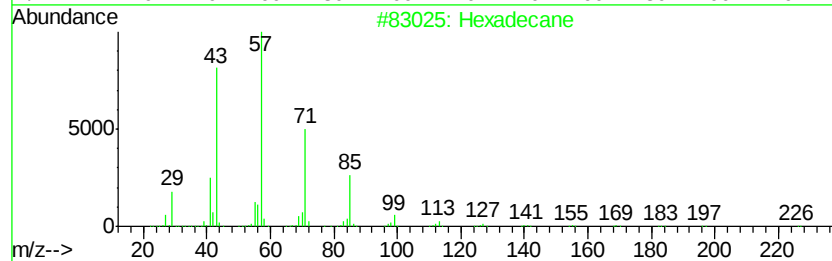
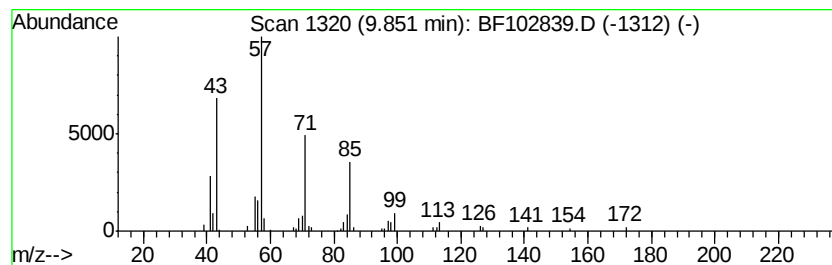
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.29 ng	147745	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	87
2	Tridecane		184	C13H28	000629-50-5	83
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80
4	Pentadecane		212	C15H32	000629-62-9	80
5	Tetradecane		198	C14H30	000629-59-4	72



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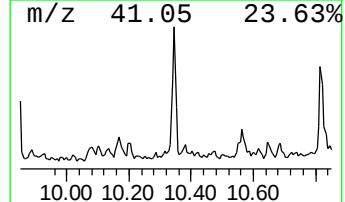
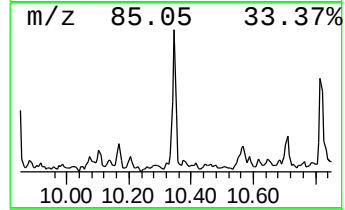
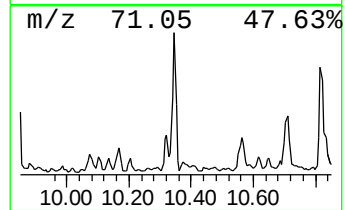
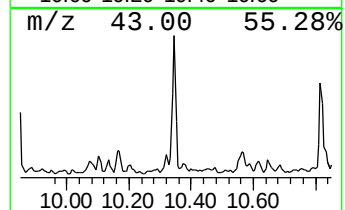
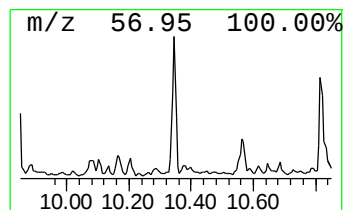
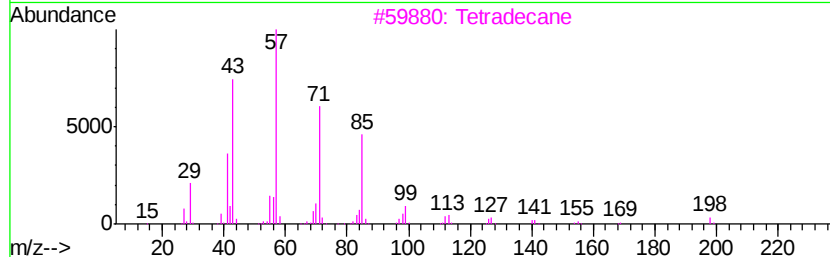
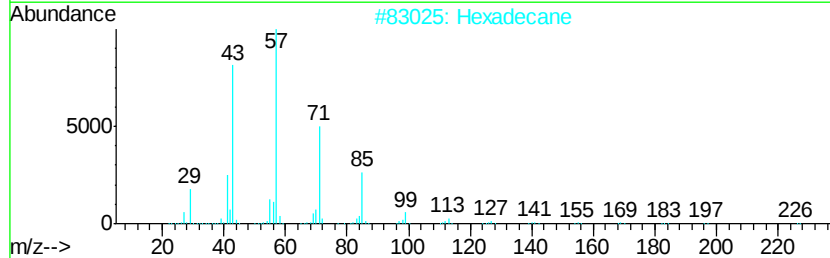
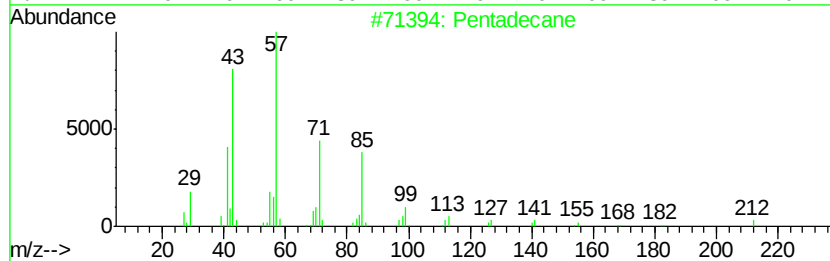
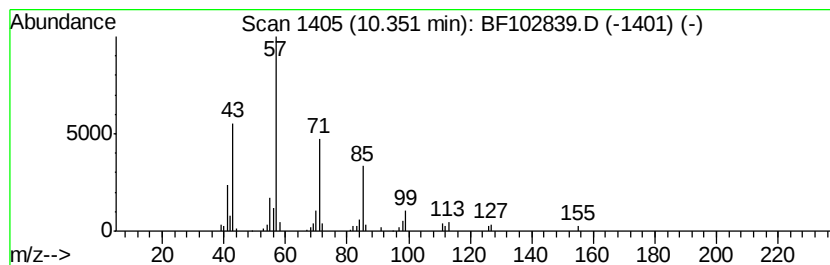
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.16 ng	139698	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	91
2	Hexadecane	226 C16H34	000544-76-3	90
3	Tetradecane	198 C14H30	000629-59-4	90
4	Heneicosane	296 C21H44	000629-94-7	80
5	Eicosane, 10-methyl-	296 C21H44	054833-23-7	78



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ALS Vial : 23 Sample Multiplier: 1

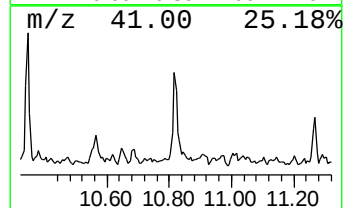
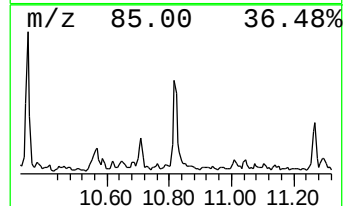
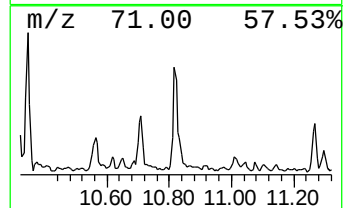
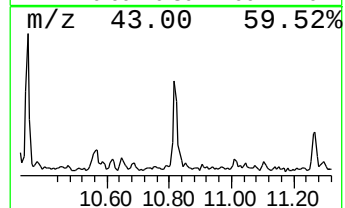
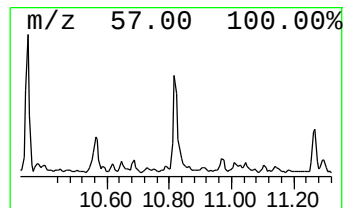
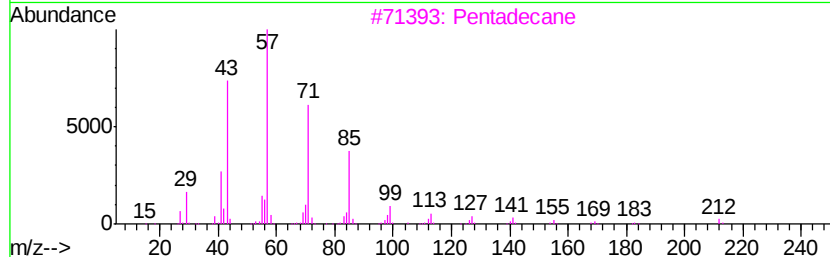
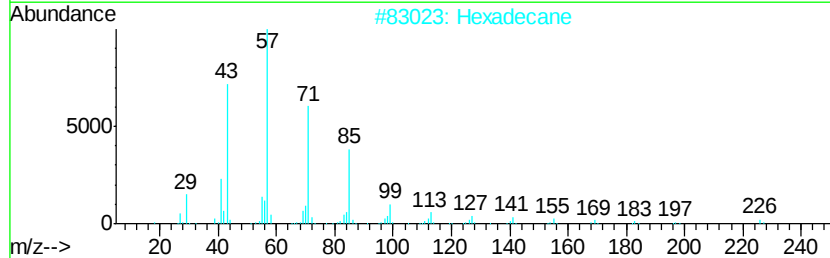
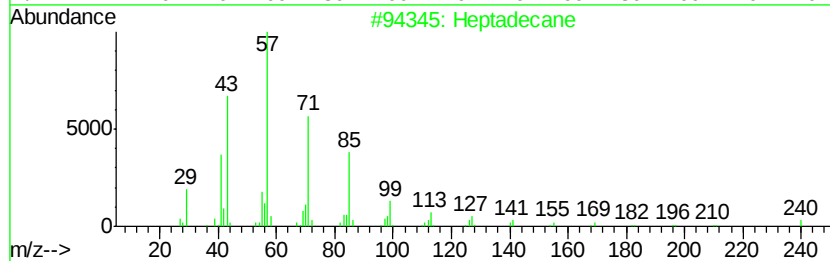
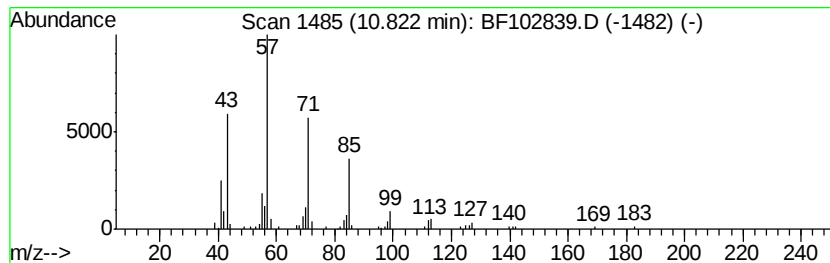
Instrument :
BNA_F
ClientSampleId :
RT-3451

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.82	2.65 ng	139973	Phenanthrene-d10	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexadecane		226	C16H34	000544-76-3	86
3	Pentadecane		212	C15H32	000629-62-9	86
4	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	80
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102839.D
Acq On : 8 Feb 2018 2:37
Operator : SJ/JU
Sample : J1465-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3451

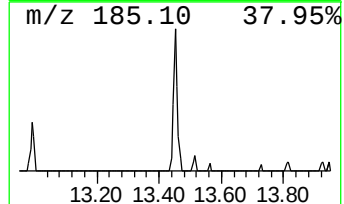
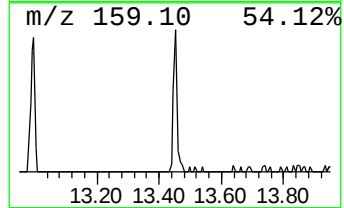
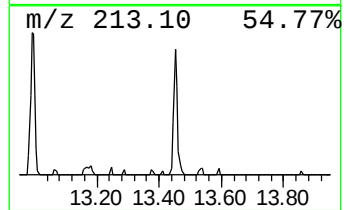
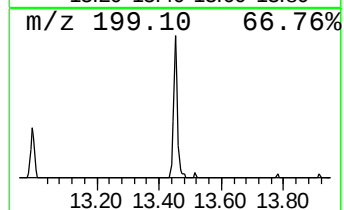
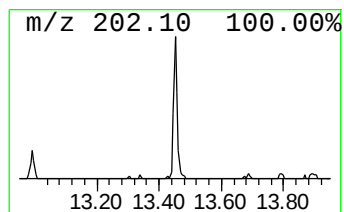
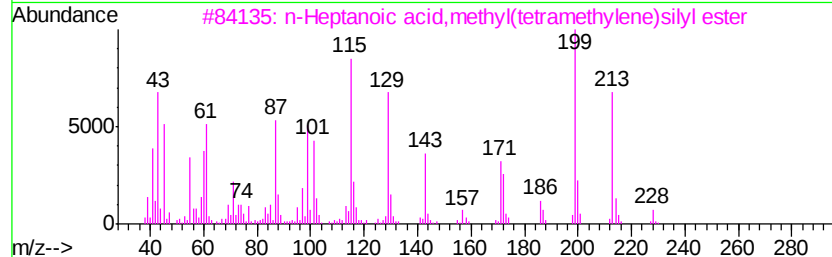
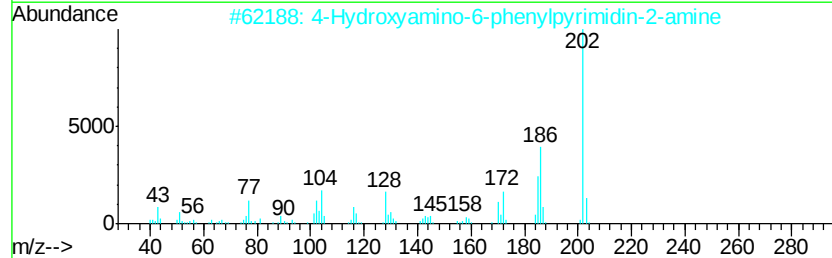
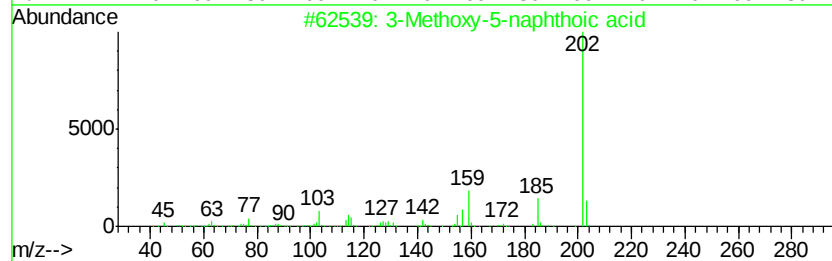
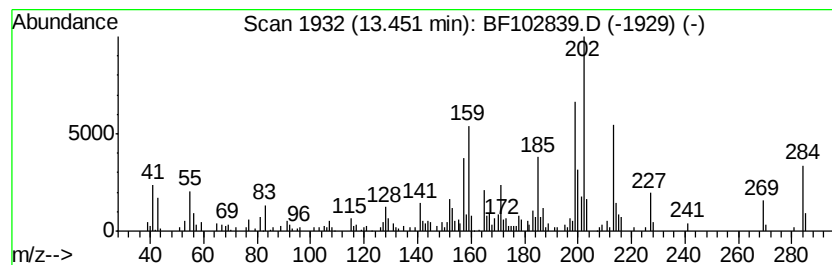
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 3-Methoxy-5-naphthoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	4.75 ng	231010	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	62
2		4-Hydroxyamino-6-phenylpyrimidin...	202	C10H10N4O	1000111-25-2	35
3		n-Heptanoic acid,methyl(tetramet...	228	C12H24O2Si	1000217-03-6	30
4		9-Borabicyclo[3.3.1]nonane, 9-br...	200	C8H14BBr	022086-45-9	20
5		4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102839.D
Acq On : 8 Feb 2018 2:37
Operator : SJ/JU
Sample : J1465-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
RT-3451

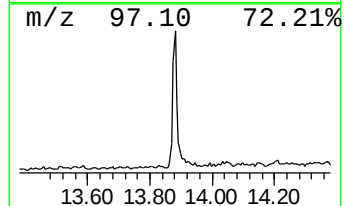
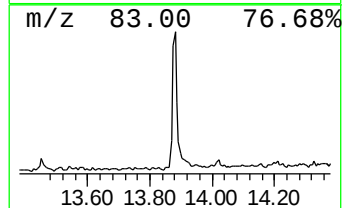
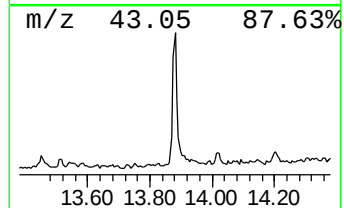
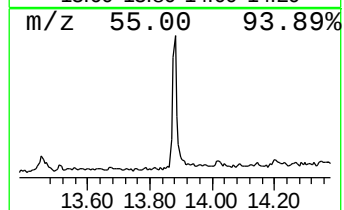
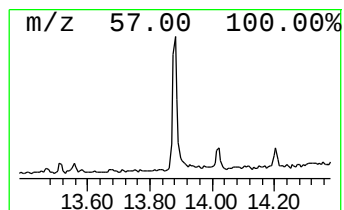
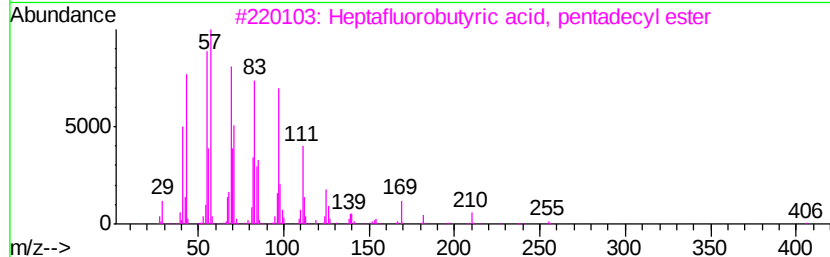
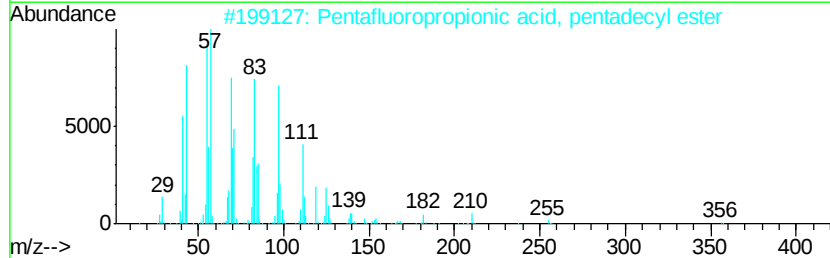
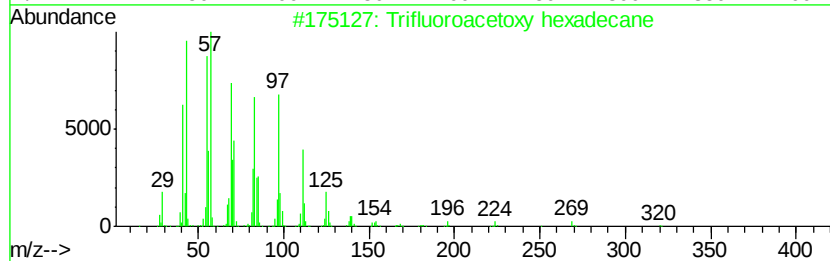
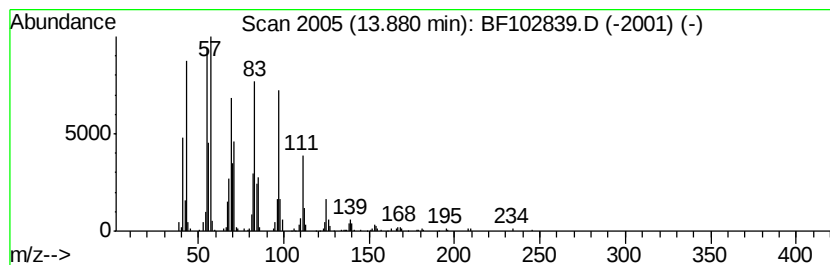
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	8.85 ng	430422	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
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Acq On : 8 Feb 2018 2:37
Operator : SJ/JU
Sample : J1465-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

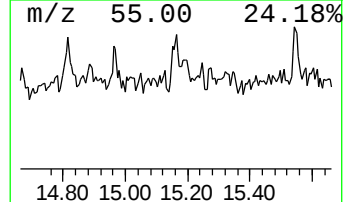
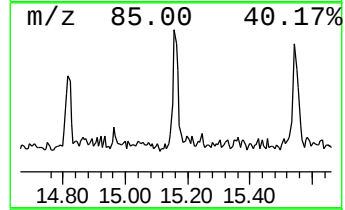
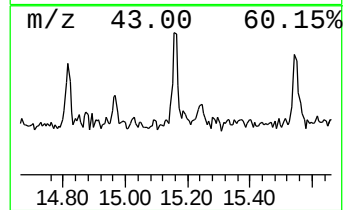
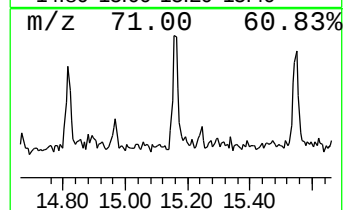
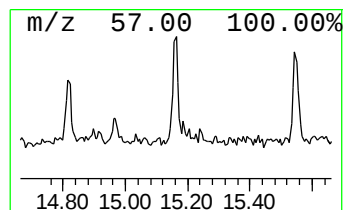
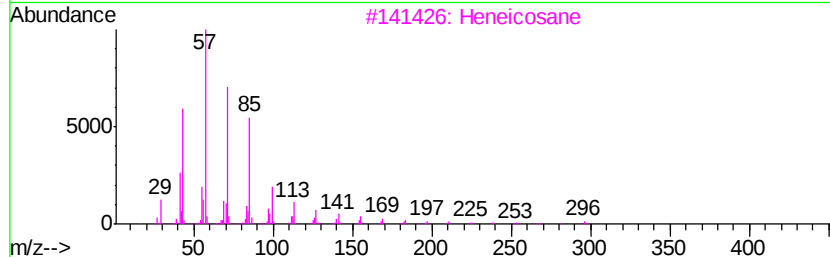
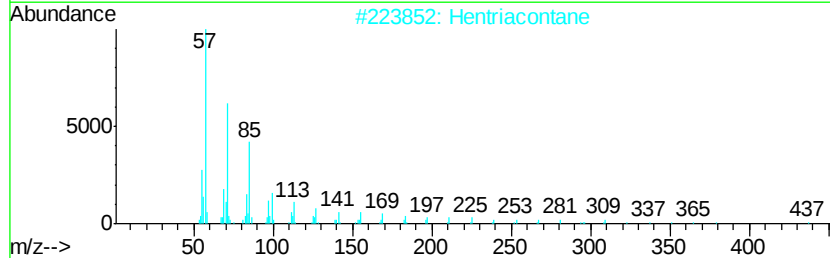
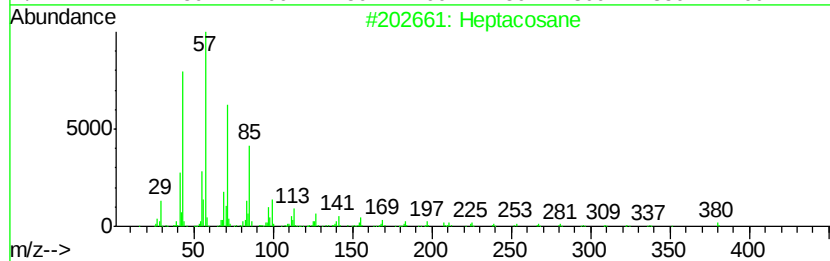
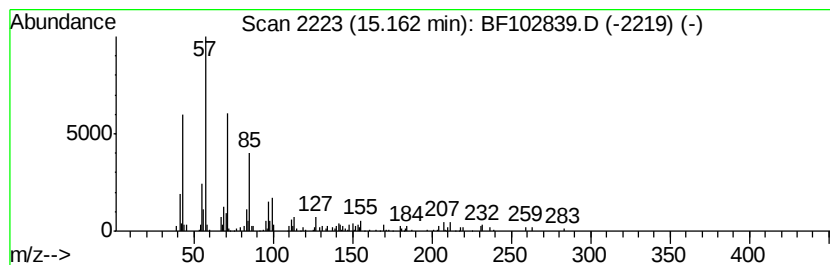
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.14 ng	91130	Perylene-d12	15.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	87
2	Hentriacontane	437 C31H64	000630-04-6	87
3	Heneicosane	296 C21H44	000629-94-7	83
4	Octacosane	394 C28H58	000630-02-4	83
5	Hexatriacontane	507 C36H74	000630-06-8	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
 Data File : BF102839.D
 Acq On : 8 Feb 2018 2:37
 Operator : SJ/JU
 Sample : J1465-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 RT-3451

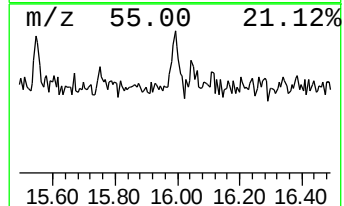
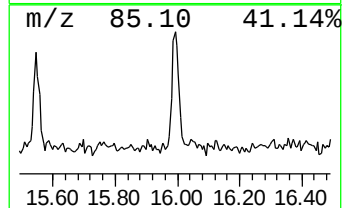
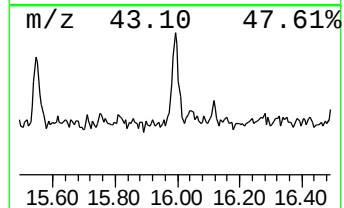
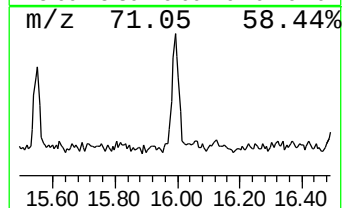
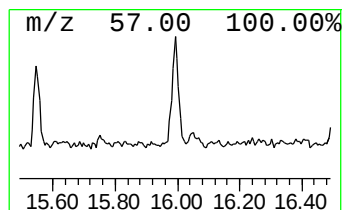
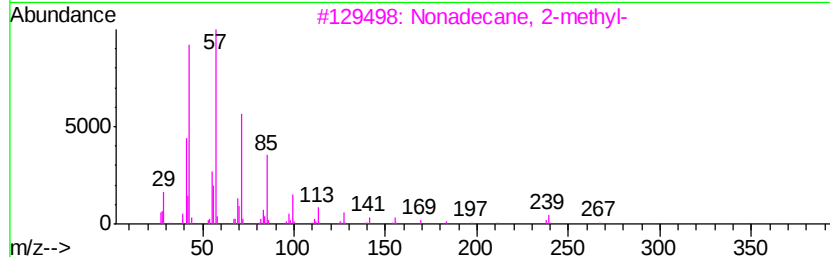
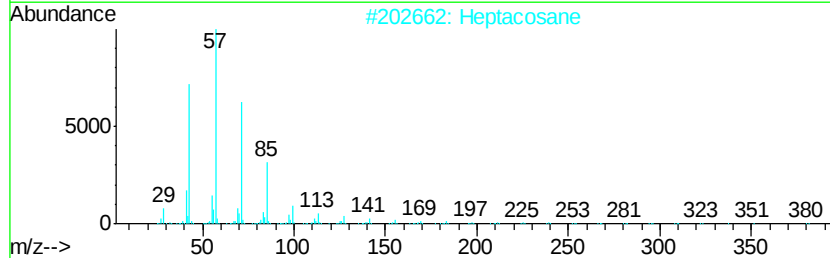
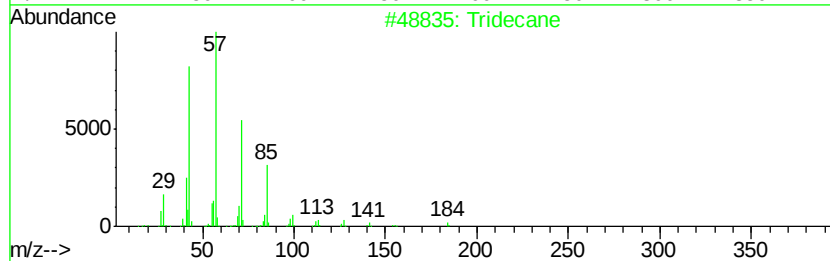
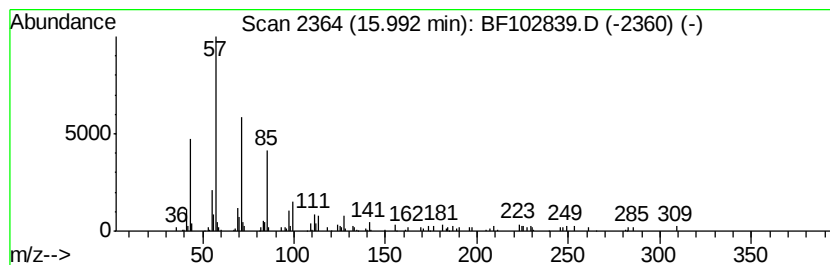
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 11 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.25 ng	96114	Perylene-d12	15.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	80
2			Heptacosane	380	C27H56	000593-49-7	80
3			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
4			13-Methylhentriacontane	451	C32H66	1000131-19-4	78
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
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Acq On : 8 Feb 2018 2:37
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3451

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	9.2	ng	513509	1	6.89	1116520	20.0
2-Pentanone, 4-hy...	5.11	3.6	ng	203623	1	6.89	1116520	20.0
unknown6.65	6.65	66.5	ng	3715160	1	6.89	1116520	20.0
Hexadecane	9.85	2.3	ng	147745	3	9.92	1292490	20.0
Pentadecane	10.35	2.2	ng	139698	3	9.92	1292490	20.0
Heptadecane	10.82	2.6	ng	139973	4	11.41	1055020	20.0
3-Methoxy-5-napht...	13.45	4.8	ng	231010	5	14.05	972514	20.0
Trifluoroacetoxy ...	13.88	8.8	ng	430422	5	14.05	972514	20.0
Heptacosane	15.16	2.1	ng	91130	6	15.53	853649	20.0
Tridecane	15.99	2.3	ng	96114	6	15.53	853649	20.0