

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082018\
 Data File : BF108307.D
 Acq On : 20 Aug 2018 23:00
 Operator : JU/SJ
 Sample : J4539-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MS-RO-27186

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.366	3	5	20	rVB	412941	482019	11.16%	1.061%
2	2.513	25	30	39	rVB	147020	217950	5.05%	0.480%
3	4.943	439	443	450	rBV	74410	113388	2.63%	0.250%
4	5.266	494	498	502	rBV	155343	183649	4.25%	0.404%
5	5.648	558	563	567	rBV	3293062	3476926	80.53%	7.656%
6	6.642	725	732	735	rBV	3214669	3655063	84.66%	8.048%
7	6.789	753	757	760	rBV	3666693	3508867	81.27%	7.726%
8	6.825	760	763	767	rVB	318083	247314	5.73%	0.545%
9	7.019	793	796	800	rVB	1173438	937758	21.72%	2.065%
10	7.078	803	806	811	rVB2	174557	165210	3.83%	0.364%
11	7.178	819	823	826	rBV	3218006	2832931	65.62%	6.238%
12	7.254	832	836	838	rBV3	146618	143153	3.32%	0.315%
13	7.531	879	883	887	rBV2	127194	169067	3.92%	0.372%
14	7.584	887	892	895	rBV	2184023	2172064	50.31%	4.782%
15	7.713	911	914	918	rVB	171429	194281	4.50%	0.428%
16	7.842	933	936	941	rVB3	153088	226214	5.24%	0.498%
17	8.031	966	968	974	rVB2	122397	127693	2.96%	0.281%
18	8.089	974	978	982	rBV2	112464	140394	3.25%	0.309%
19	8.131	982	985	988	rBV	200006	197012	4.56%	0.434%
20	8.301	1009	1014	1017	rBV	1202774	1116465	25.86%	2.458%
21	8.325	1017	1018	1022	rVB3	230995	189969	4.40%	0.418%
22	8.372	1022	1026	1029	rBV4	91919	154003	3.57%	0.339%
23	8.413	1029	1033	1035	rBV2	113779	153775	3.56%	0.339%
24	8.513	1046	1050	1054	rBV5	84406	159718	3.70%	0.352%
25	8.613	1065	1067	1070	rBV3	128566	143731	3.33%	0.316%
26	8.666	1072	1076	1078	rVV	237689	280017	6.49%	0.617%
27	8.695	1078	1081	1084	rVV2	137727	179534	4.16%	0.395%
28	8.766	1091	1093	1096	rBV3	246511	267096	6.19%	0.588%
29	8.801	1096	1099	1101	rVV	597174	461907	10.70%	1.017%
30	8.825	1101	1103	1105	rVV2	220218	201523	4.67%	0.444%
31	8.860	1107	1109	1111	rVV2	482484	549185	12.72%	1.209%
32	8.901	1114	1116	1118	rVV2	343297	290913	6.74%	0.641%
33	8.925	1118	1120	1122	rVB	273664	198638	4.60%	0.437%
34	8.966	1123	1127	1130	rVB3	495374	625847	14.50%	1.378%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.019	1131	1136	1138	rBV3	324855	568563	13.17%	1.252%
36	9.048	1138	1141	1144	rBV3	303961	395261	9.15%	0.870%
37	9.201	1165	1167	1171	rBV4	374149	527271	12.21%	1.161%
38	9.266	1175	1178	1181	rBV2	834759	1032177	23.91%	2.273%
39	9.342	1189	1191	1193	rVB2	623465	469081	10.86%	1.033%
40	9.378	1193	1197	1200	rBV	3681968	3631292	84.11%	7.995%
41	9.566	1225	1229	1232	rVB3	1325337	1472414	34.10%	3.242%
42	9.613	1235	1237	1240	rBV3	423442	473069	10.96%	1.042%
43	9.772	1261	1264	1266	rBV3	728341	622901	14.43%	1.372%
44	9.925	1287	1290	1292	rBV2	610618	689139	15.96%	1.517%
45	10.019	1303	1306	1310	rBV2	616222	995803	23.06%	2.193%
46	10.072	1312	1315	1317	rVB2	1128536	1171936	27.14%	2.580%
47	10.930	1458	1461	1465	rBV	1609030	2290983	53.06%	5.044%
48	11.083	1485	1487	1492	rVB	2103373	2596372	60.14%	5.717%
49	11.519	1556	1561	1565	rBV2	2131905	4317434	100.00%	9.506%

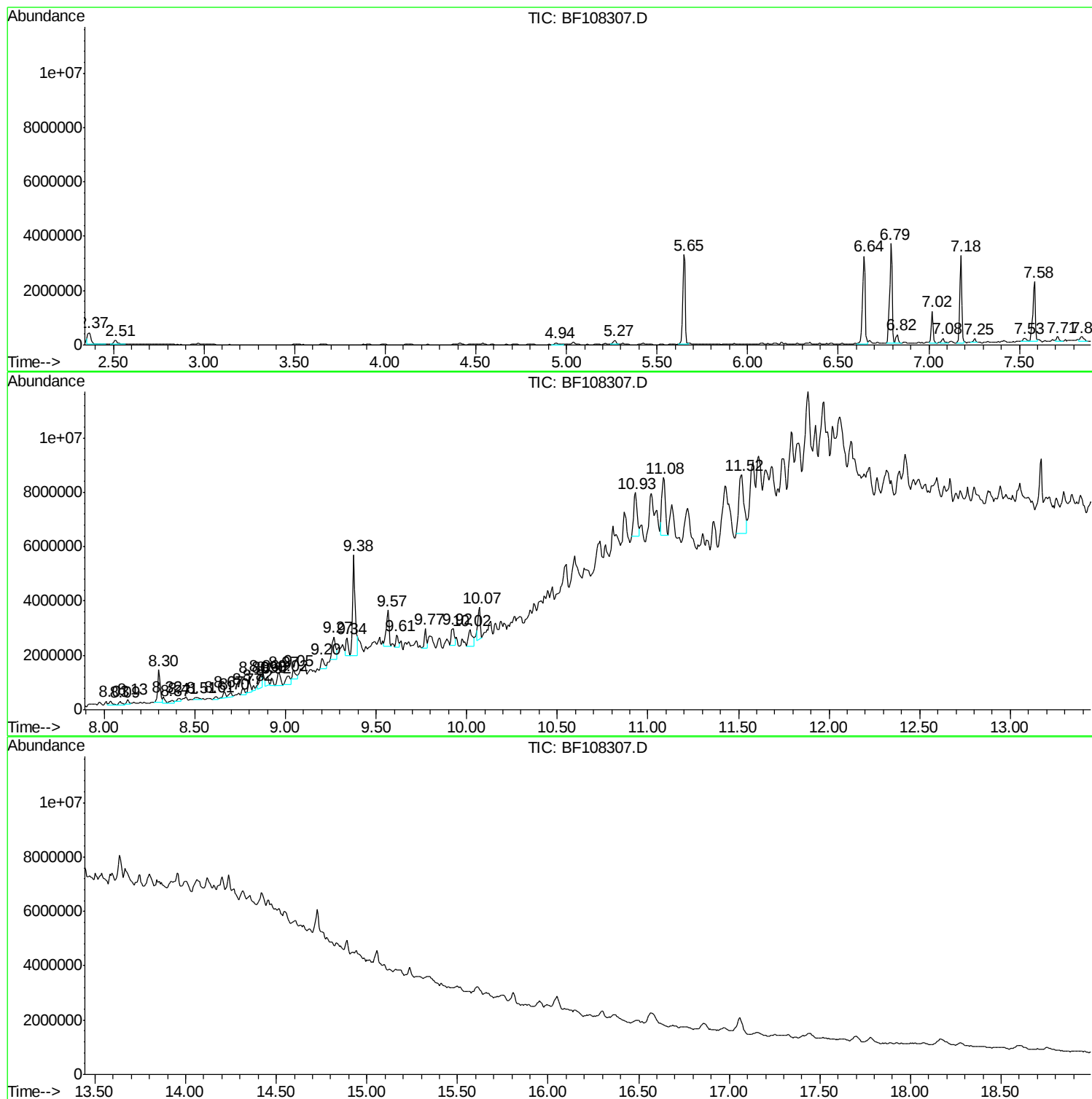
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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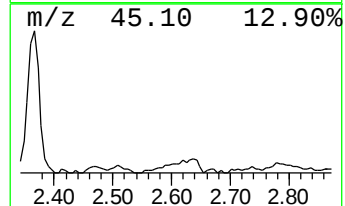
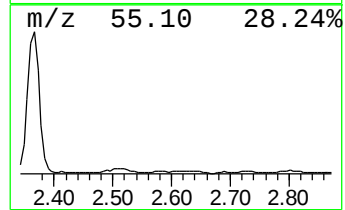
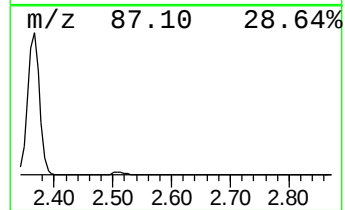
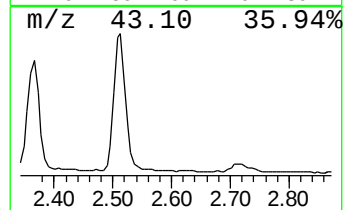
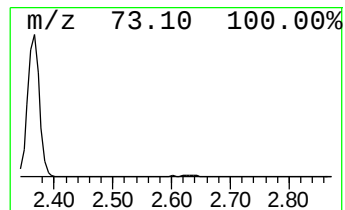
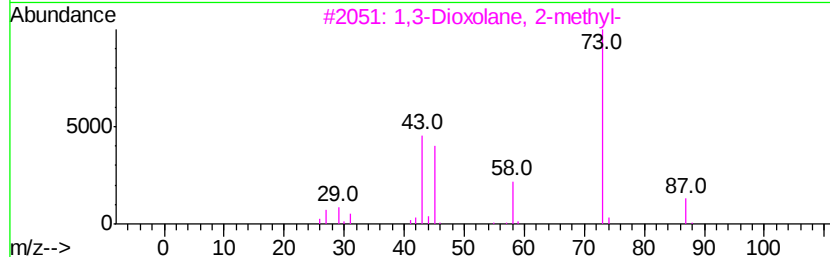
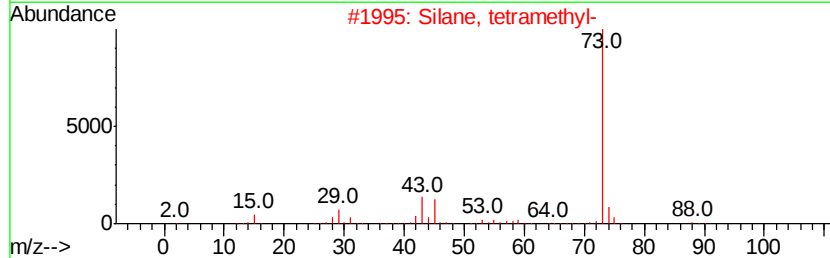
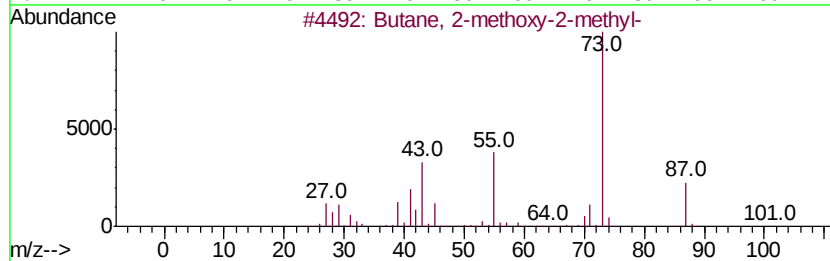
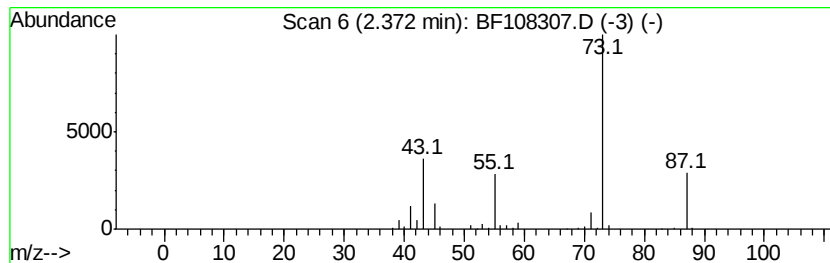
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
2.37	10.28 ng	482019	1,4-Dichlorobenzene-d4		7.02		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	12
5			Borane, dimethoxy-	74	C2H7B02	004542-61-4	9



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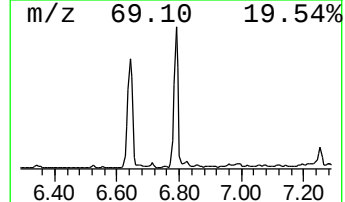
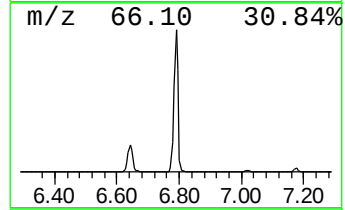
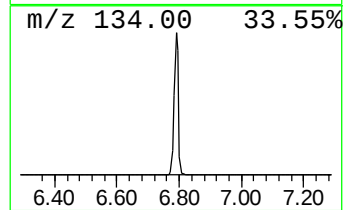
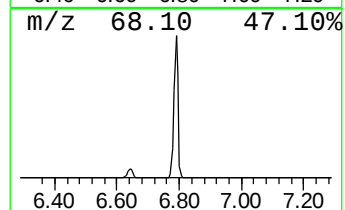
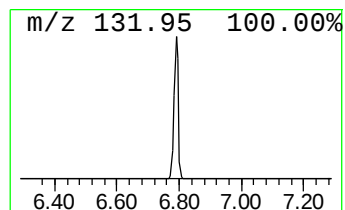
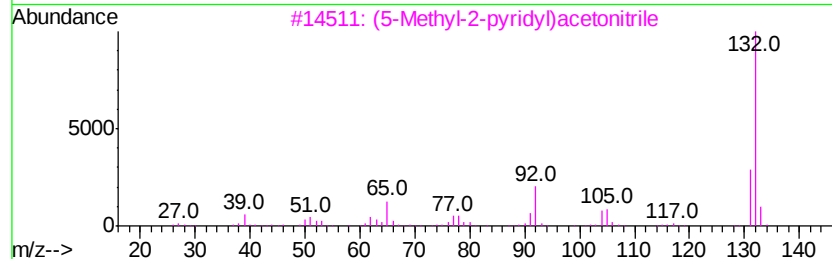
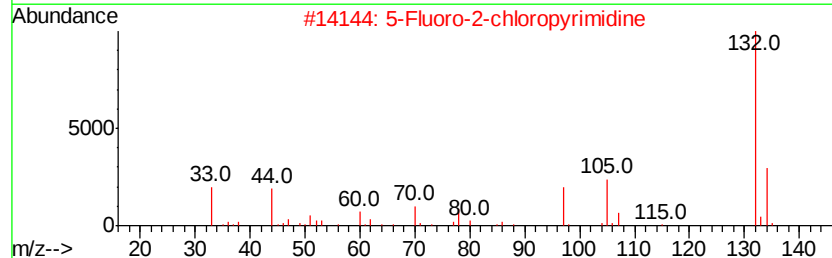
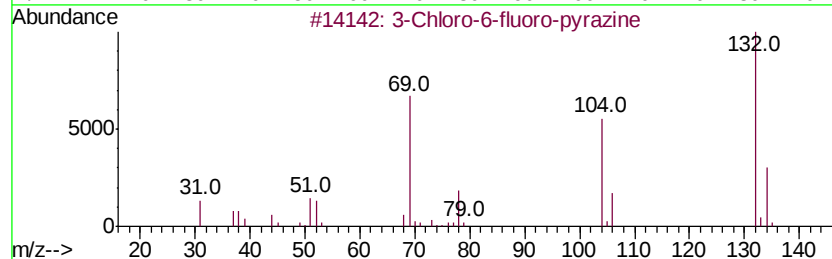
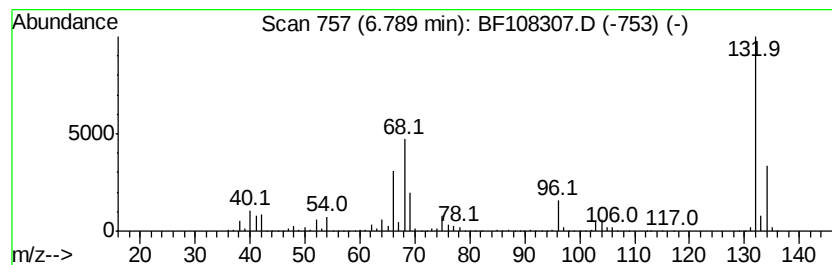
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	74.84 ng	3508870	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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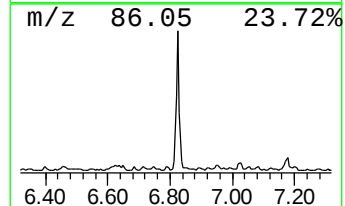
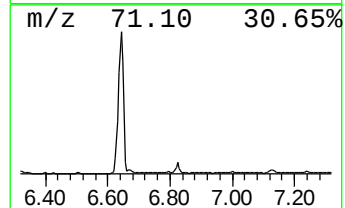
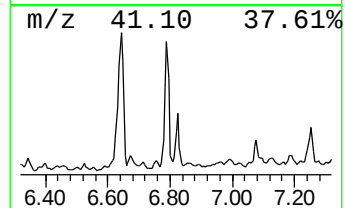
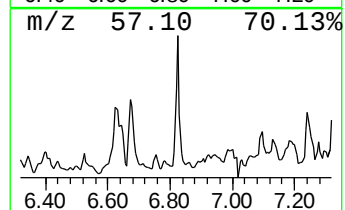
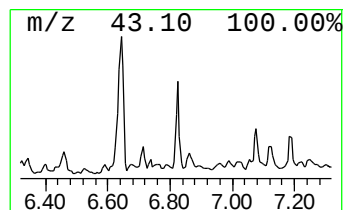
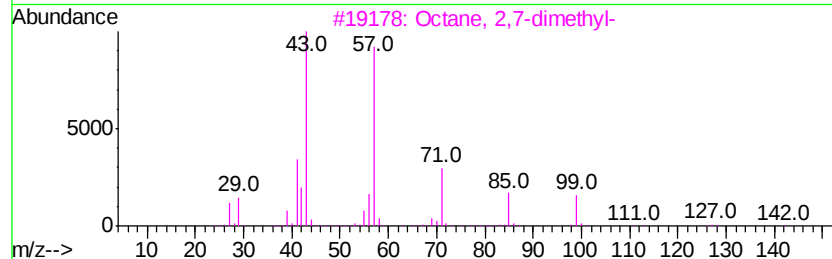
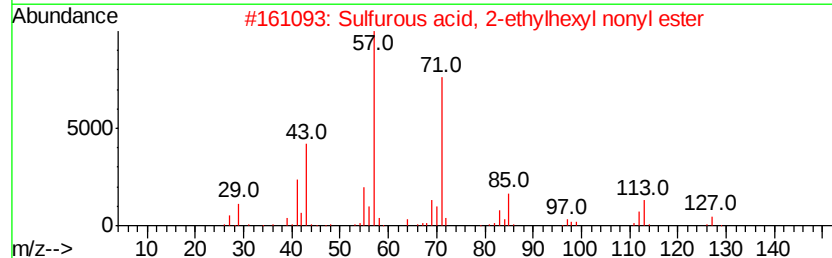
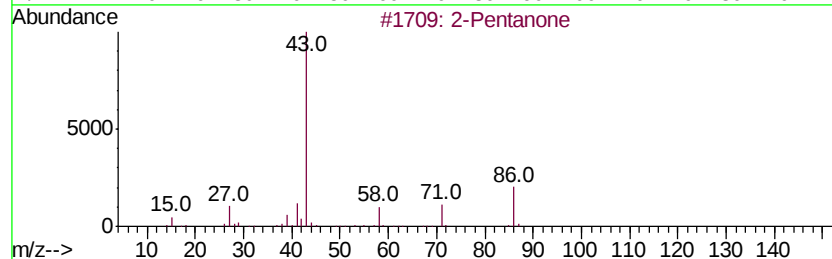
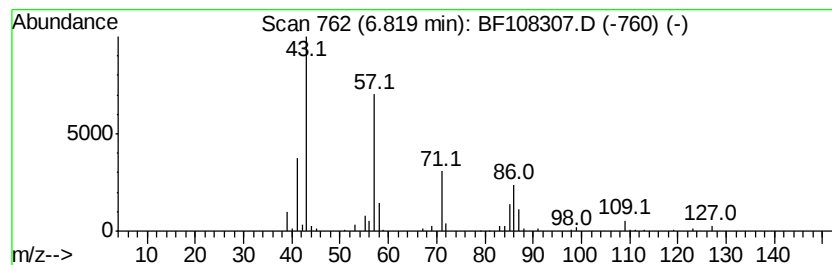
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.82 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	5.27 ng	247314	1,4-Dichlorobenzene-d4	7.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	46
2			Sulfurous acid, 2-ethylhexyl nonyl ester	320	C17H36O3S	1000309-19-2	25
3			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	25
4			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	25
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	25



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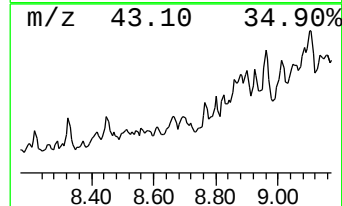
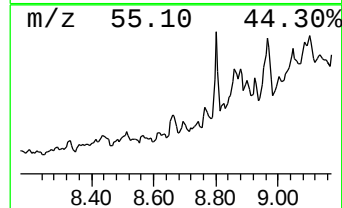
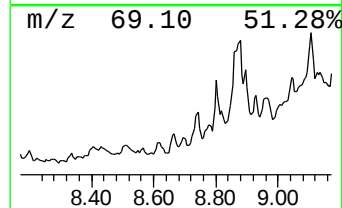
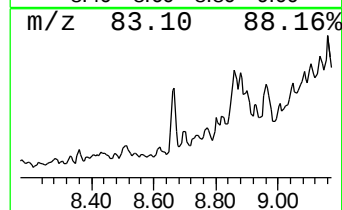
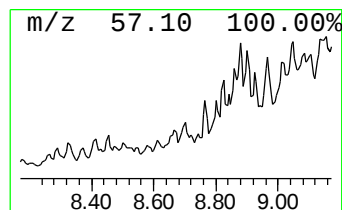
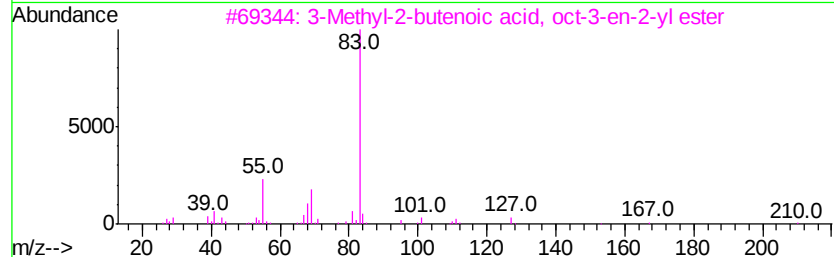
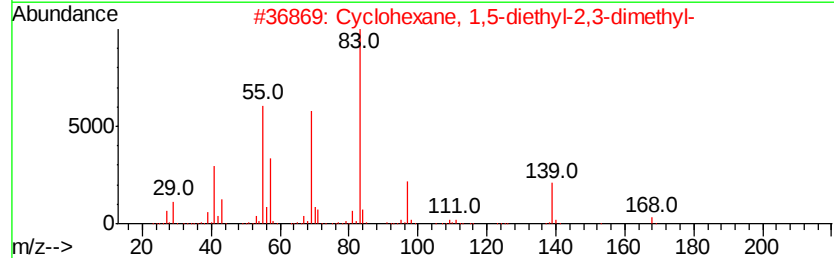
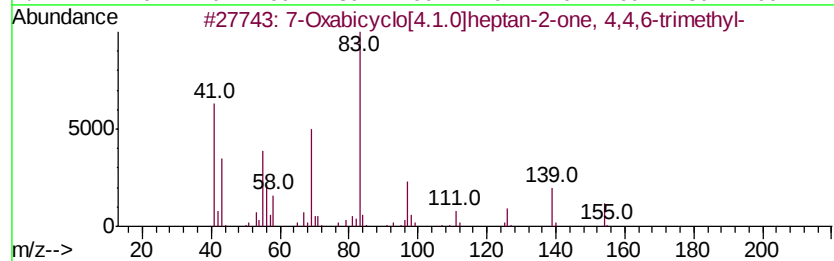
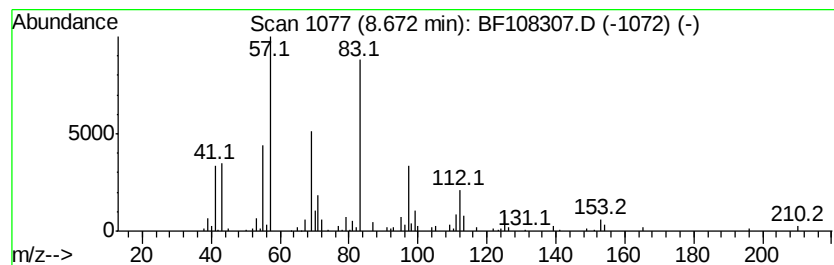
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7-Oxabicyclo[4.1.0]heptan-2... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.67	5.02 ng	280017	Naphthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Oxabicyclo[4.1.0]heptan-2-one,...	154	C9H14O2	010276-21-8	72
2		Cyclohexane, 1,5-diethyl-2,3-dim...	168	C12H24	074663-66-4	64
3		3-Methyl-2-butenic acid, oct-3-...	210	C13H22O2	1000299-31-2	50
4		1,5-Heptadien-4-one, 3,3,6-trime...	152	C10H16O	000546-49-6	47
5		4-Hexen-3-one, 5-methyl-	112	C7H12O	013905-10-7	47



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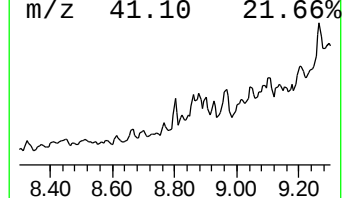
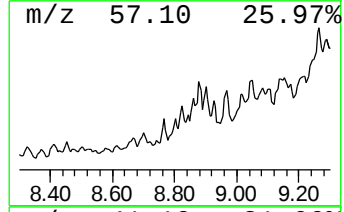
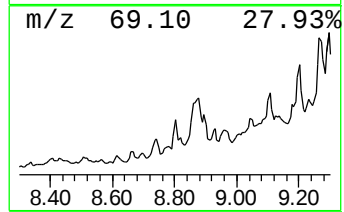
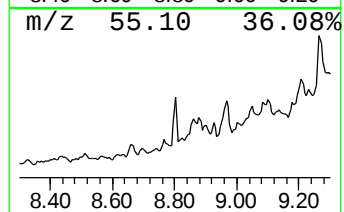
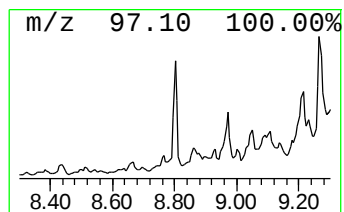
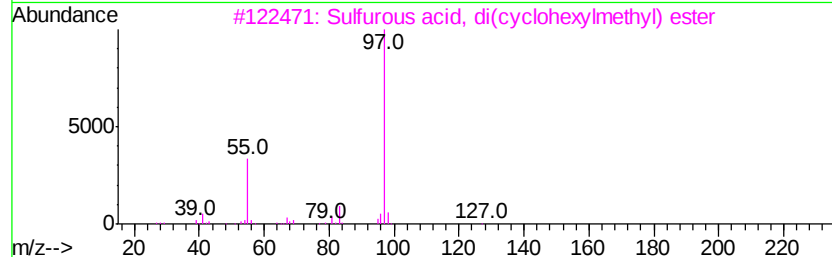
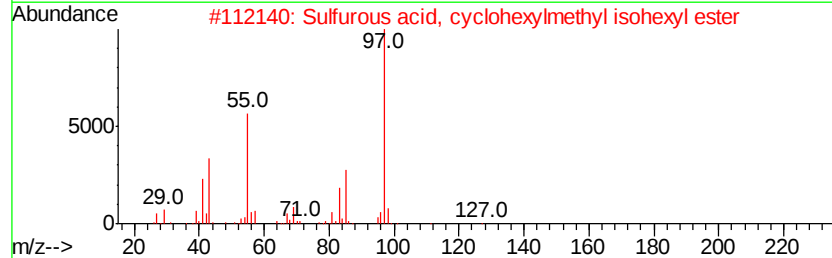
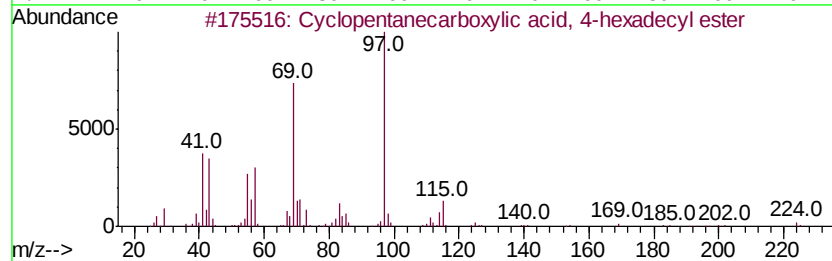
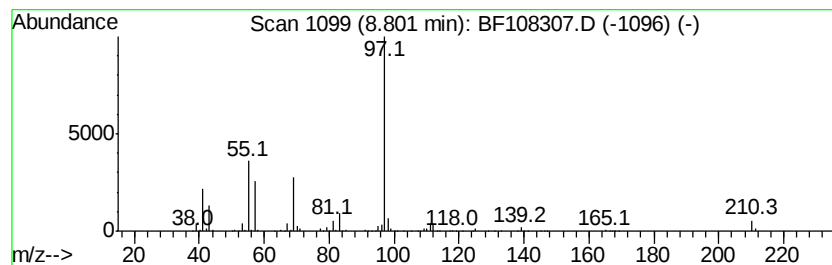
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ClientSampleId :
MS-RO-27186

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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 6 Cyclopentanecarboxylic acid... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	8.27 ng	461907	Naphthalene-d8	8.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentanecarboxylic acid, 4-h...	338 C22H42O2	1000282-77-5 64
2		Sulfurous acid, cyclohexylmethyl...	262 C13H26O3S	1000309-21-5 64
3		Sulfurous acid, di(cyclohexylmet...	274 C14H26O3S	1000309-22-7 50
4		1H-Pyrazole, 5-ethyl-4,5-dihydro...	126 C7H14N2	021981-22-6 50
5		Sulfurous acid, cyclohexylmethyl...	402 C23H46O3S	1000309-22-4 50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-RO-27186

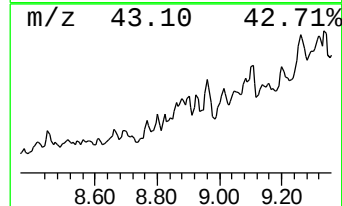
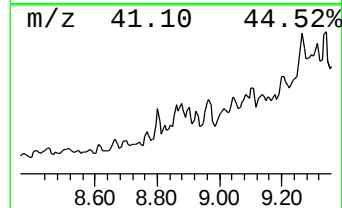
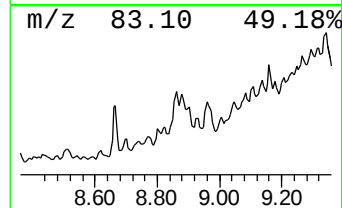
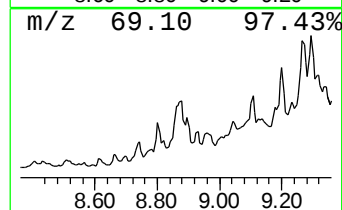
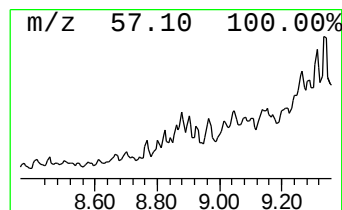
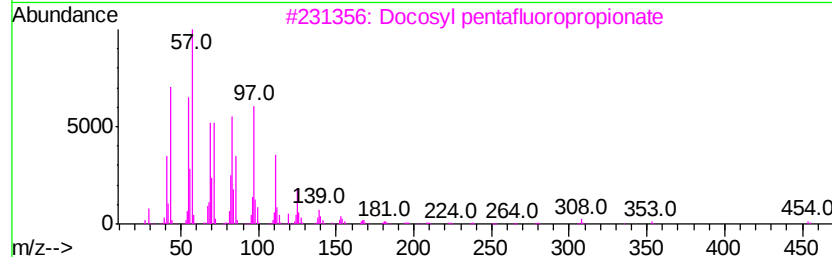
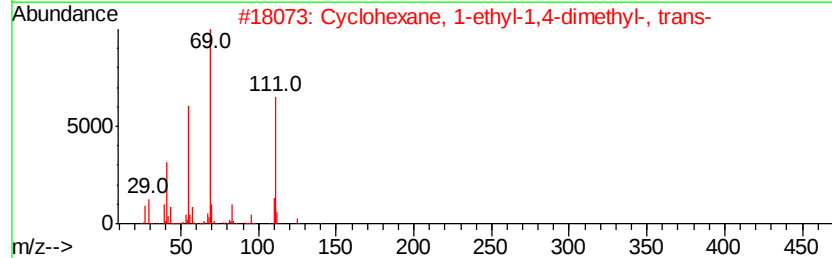
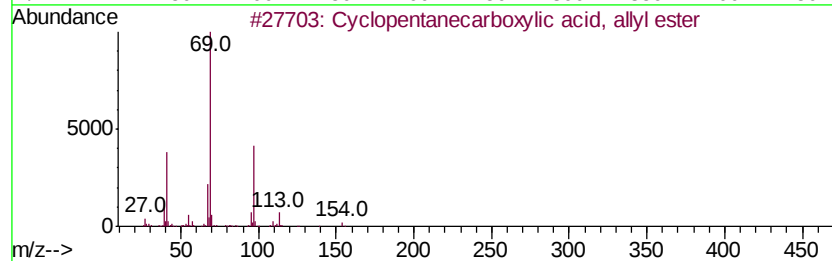
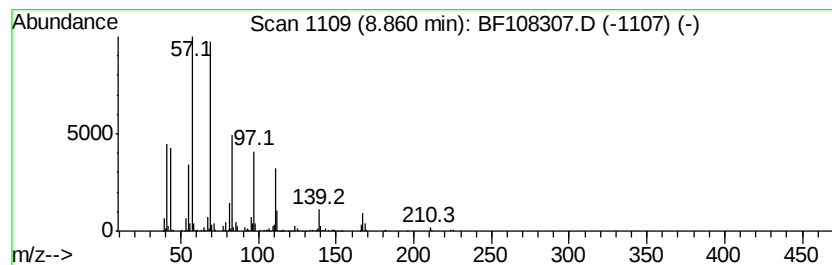
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.86 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.86	9.84 ng	549185	Napthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentanecarboxylic acid, all...	154	C9H14O2	178905-33-4	38
2		Cyclohexane, 1-ethyl-1,4-dimethy...	140	C10H20	062238-32-8	38
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	37
4		Cyclooctanemethanol	142	C9H18O	003637-63-6	25
5		Cyclopentanecarboxylic acid, 3-f...	208	C12H13F02	1000331-07-2	23



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
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ClientSampleId :
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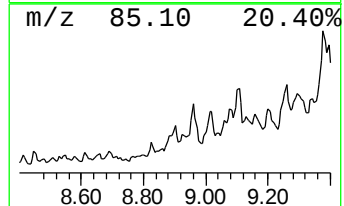
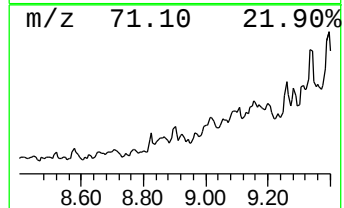
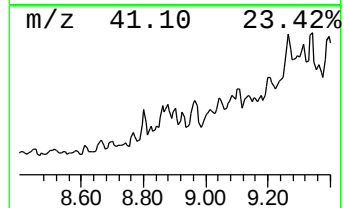
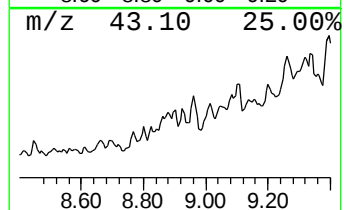
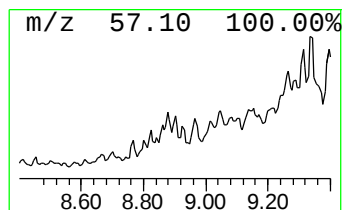
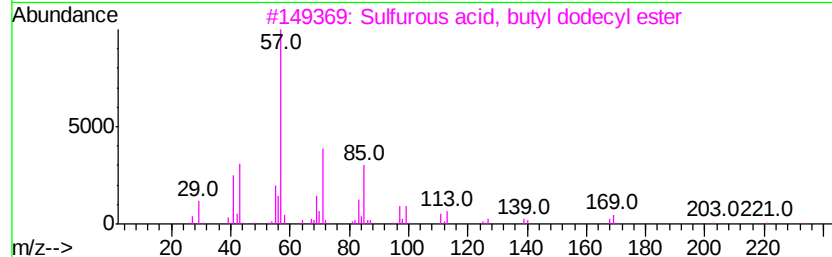
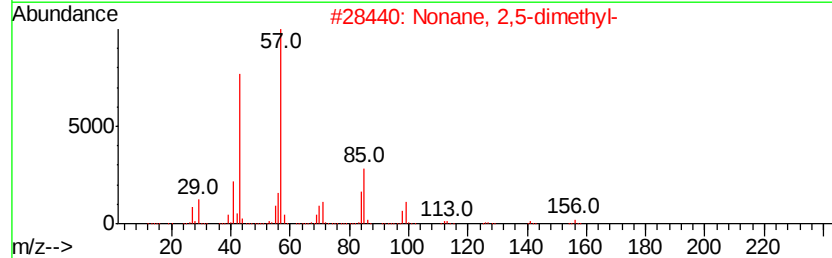
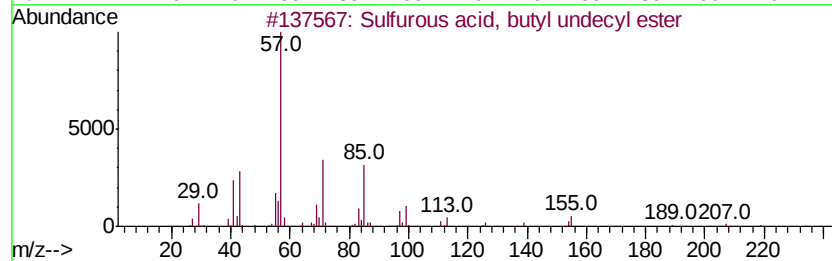
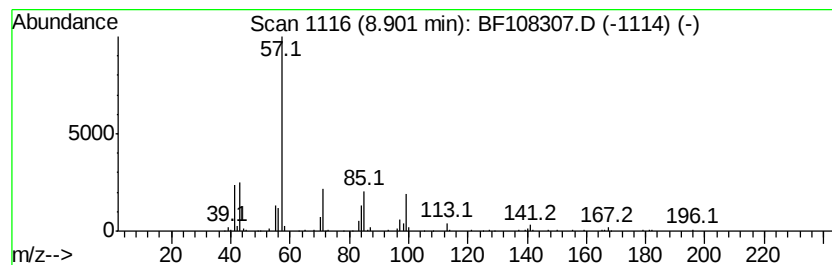
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, butyl undec... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	5.21 ng	290913	Napthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	53
2		Nonane, 2,5-dimethyl-	156	C11H24	017302-27-1	47
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	47
4		Octacosane	394	C28H58	000630-02-4	47
5		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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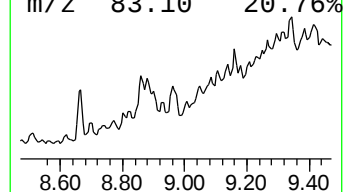
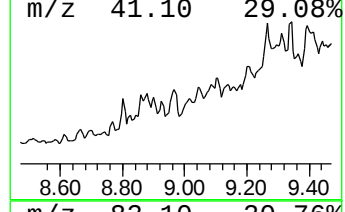
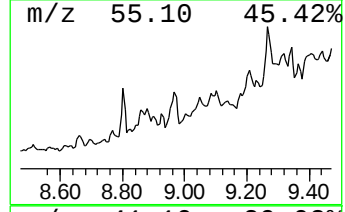
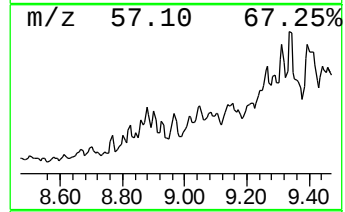
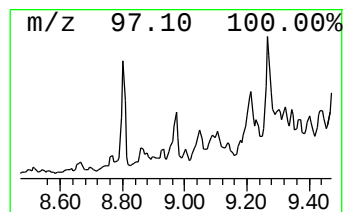
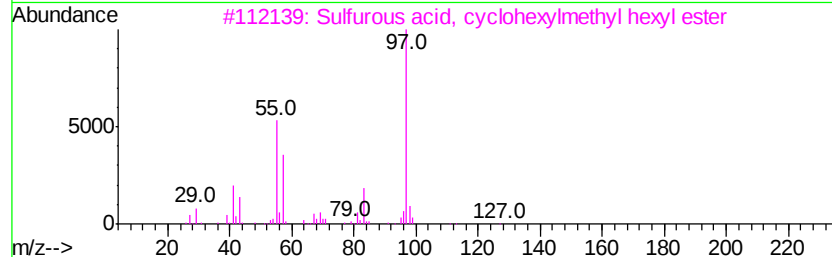
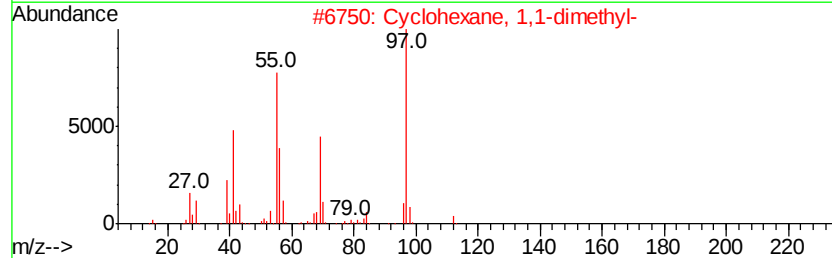
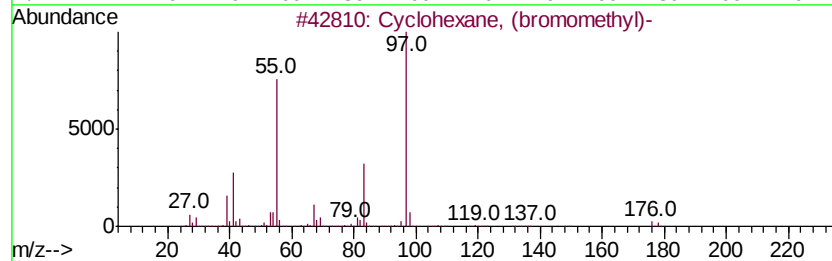
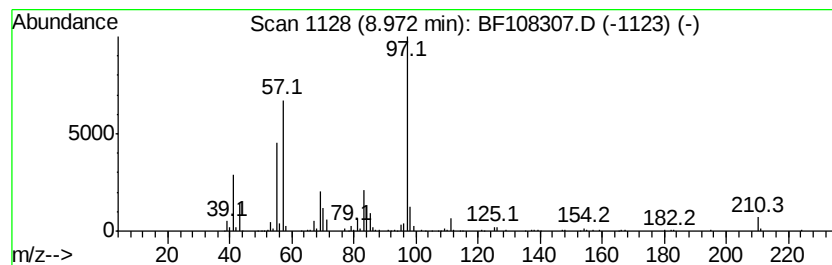
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	11.21 ng	625847	Naphthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	43
2		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	38
3		Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	37
4		Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
5		2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
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Misc :
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Instrument :
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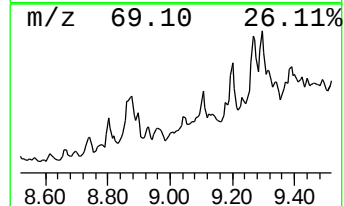
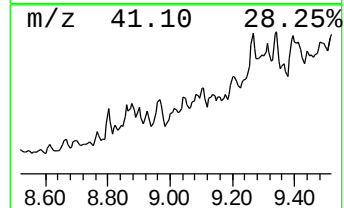
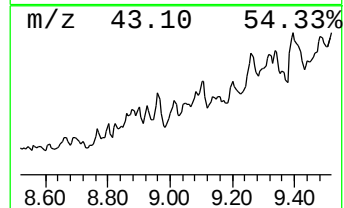
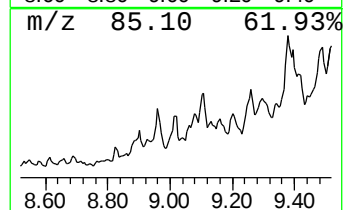
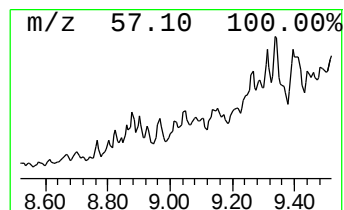
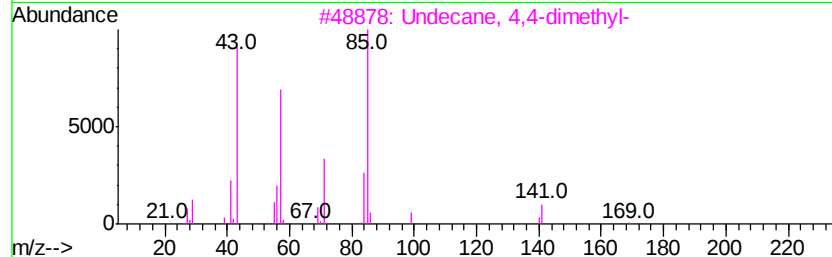
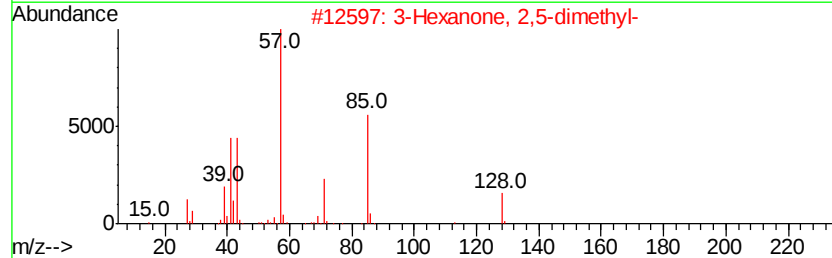
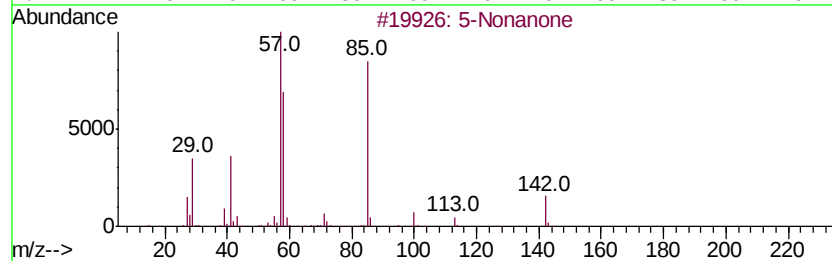
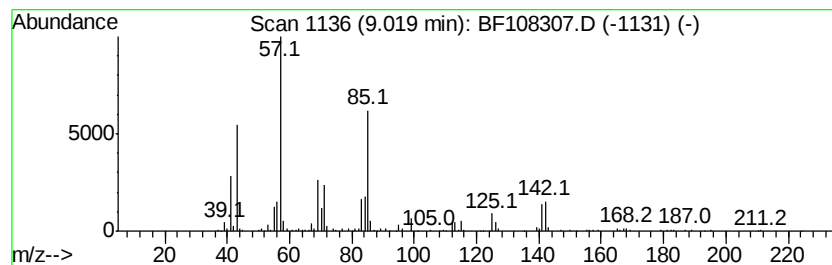
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.02 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	10.19 ng	568563	Napthalene-d8	8.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nonanone			142	C9H18O	000502-56-7	49
2	3-Hexanone, 2,5-dimethyl-			128	C8H16O	001888-57-9	47
3	Undecane, 4,4-dimethyl-			184	C13H28	017312-68-4	47
4	Sulfurous acid, butyl isohexyl e...			222	C10H22O3S	1000309-17-2	38
5	4-Heptanone, 2,6-dimethyl-			142	C9H18O	000108-83-8	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-RO-27186

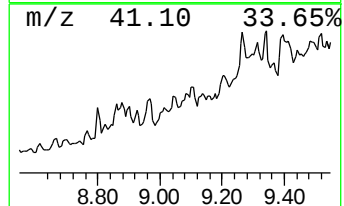
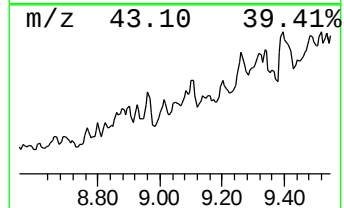
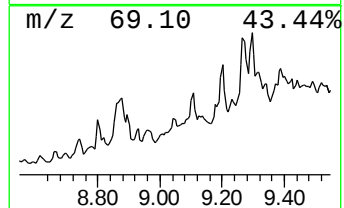
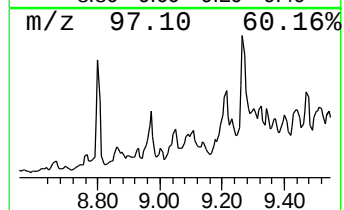
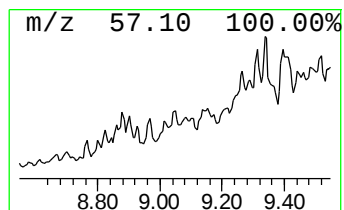
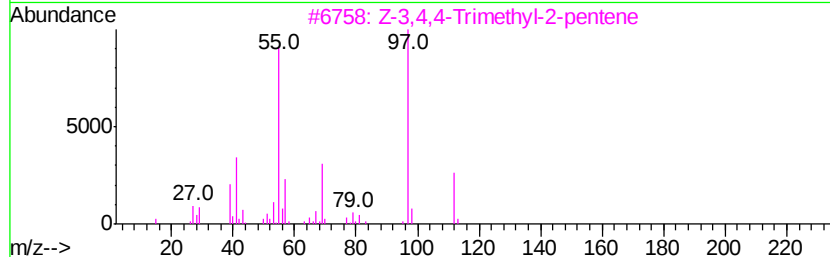
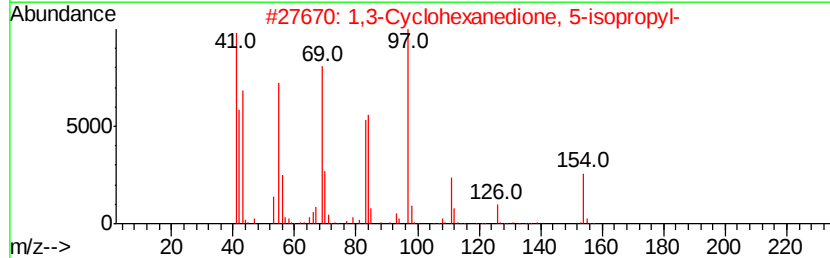
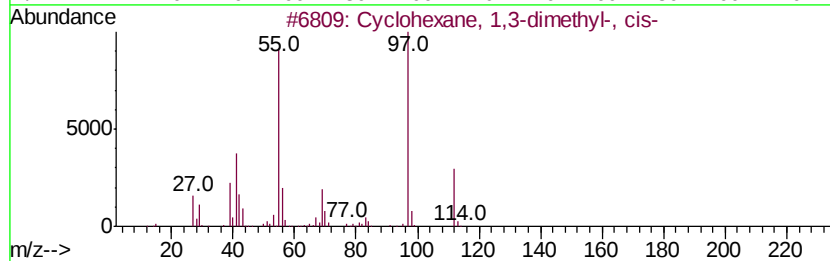
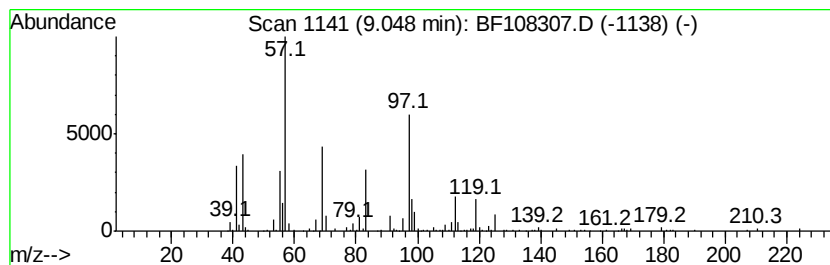
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.05 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	7.08 ng	395261	Naphthalene-d8	8.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	35
2			1,3-Cyclohexanedione, 5-isopropyl-	154	C9H14O2	018456-87-6	32
3			Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	32
4			Cyclohexene, 1-(1,1-dimethyletho...	168	C11H20O	040648-24-6	27
5			Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

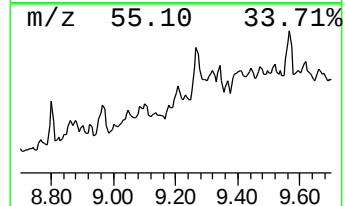
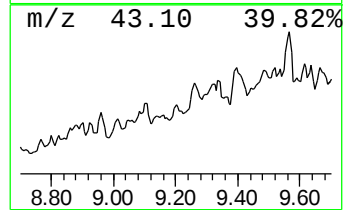
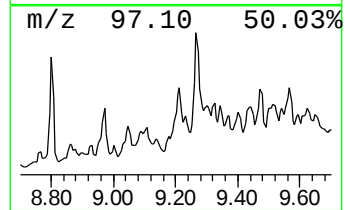
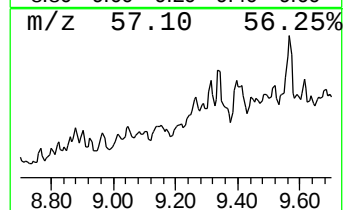
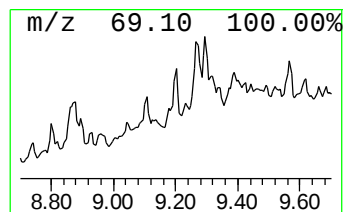
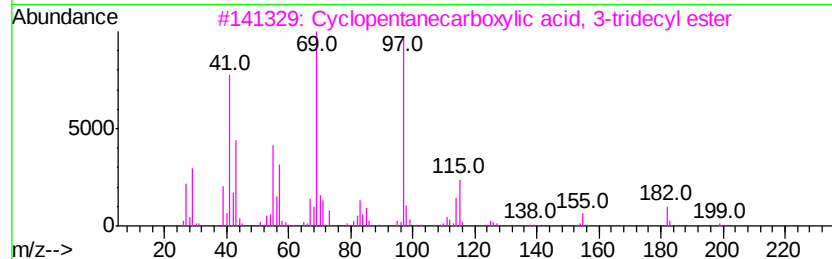
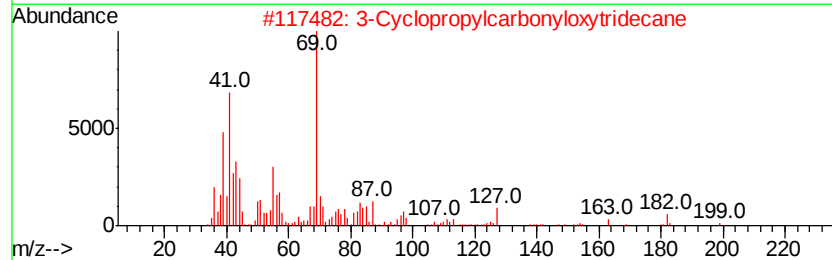
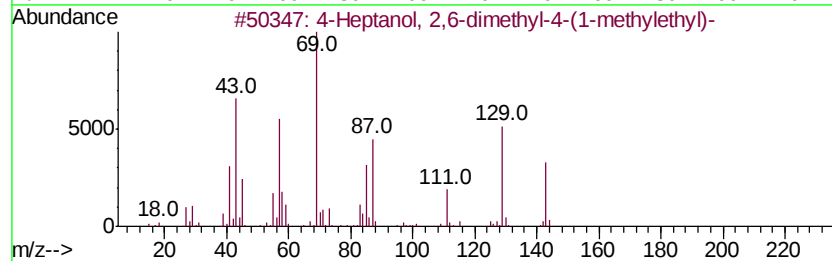
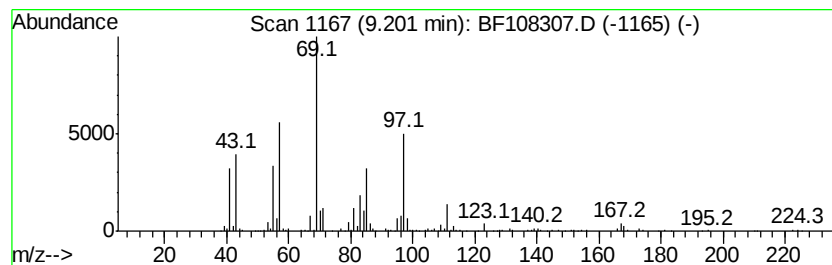
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4-Heptanol, 2,6-dimethyl-4-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.20	9.00 ng	527271	Acenaphthene-d10	10.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-4-(1-me...	186	C12H26O	054775-01-8	50
2	3-Cyclopropylcarbonyloxytridecane	268	C17H32O2	1000245-58-4	47
3	Cyclopentanecarboxylic acid, 3-t...	296	C19H36O2	1000280-58-5	45
4	Oxirane, (1,1-dimethylbutyl)-	128	C8H16O	053907-76-9	43
5	5-Hexadecanol	242	C16H34O	021078-87-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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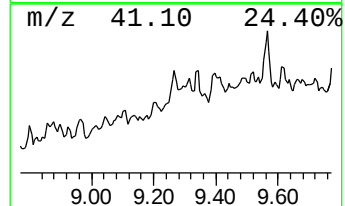
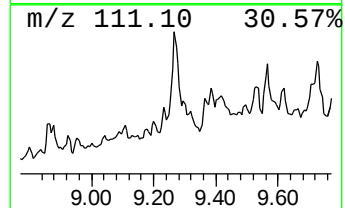
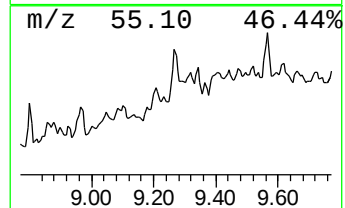
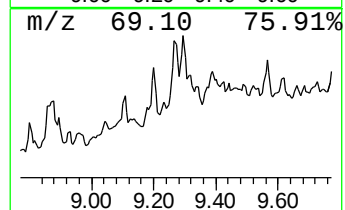
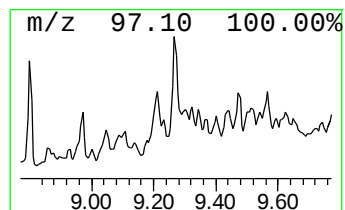
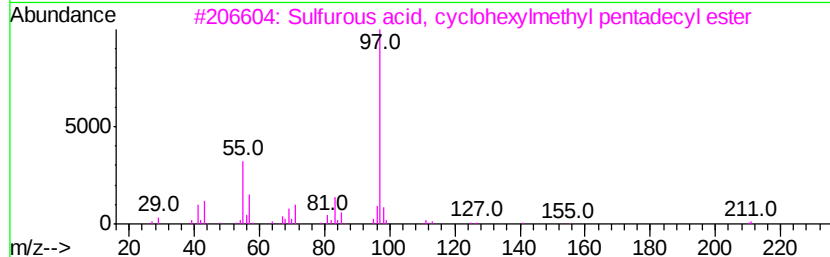
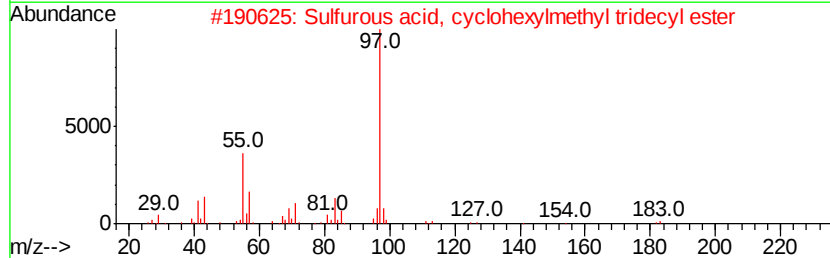
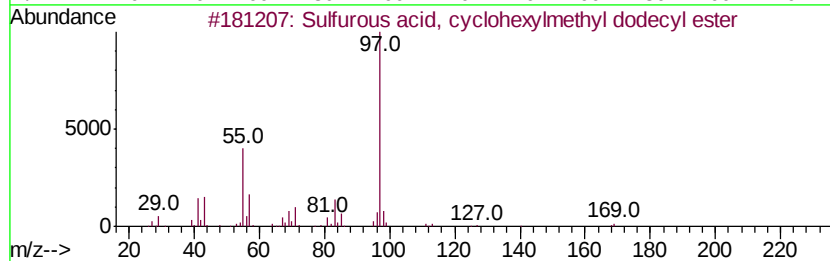
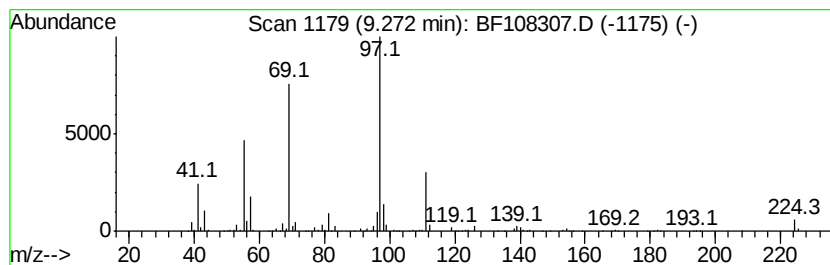
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Sulfurous acid, cyclohexylm... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	17.61 ng	1032180	Acenaphthene-d10	10.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, cvclohexylmethyl...	346	C19H38O3S	1000309-22-0	64
2		Sulfurous acid, cvclohexylmethyl...	360	C20H40O3S	1000309-22-1	64
3		Sulfurous acid, cvclohexylmethyl...	388	C22H44O3S	1000309-22-3	59
4		Sulfurous acid, cvclohexylmethyl...	332	C18H36O3S	1000309-21-9	59
5		Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
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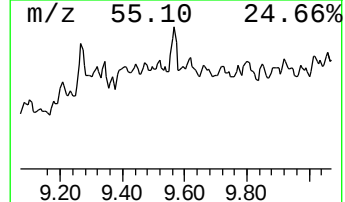
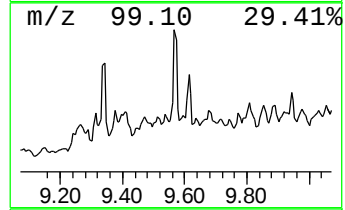
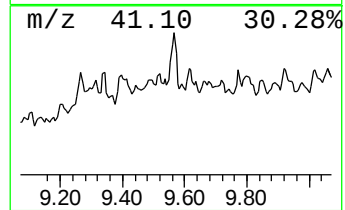
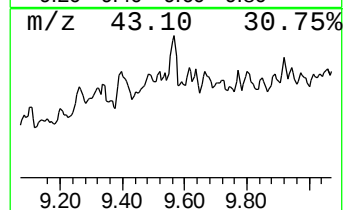
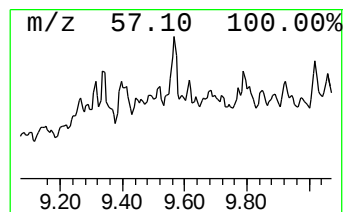
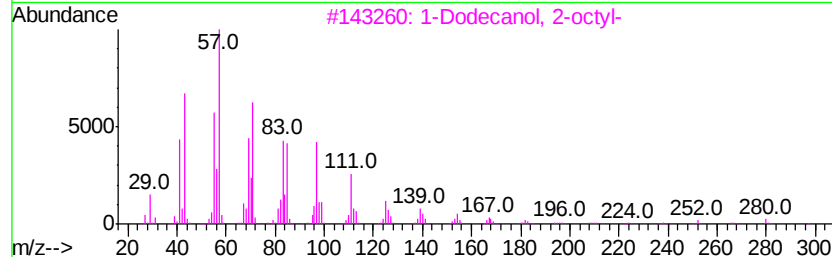
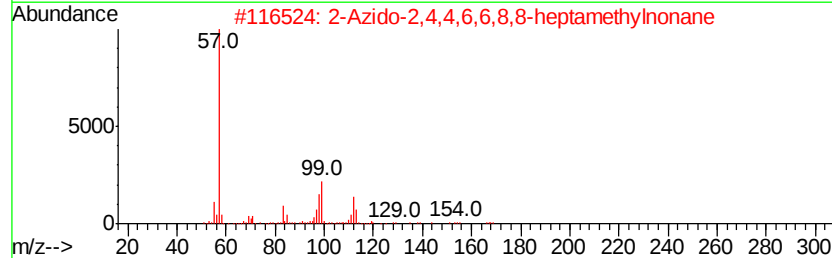
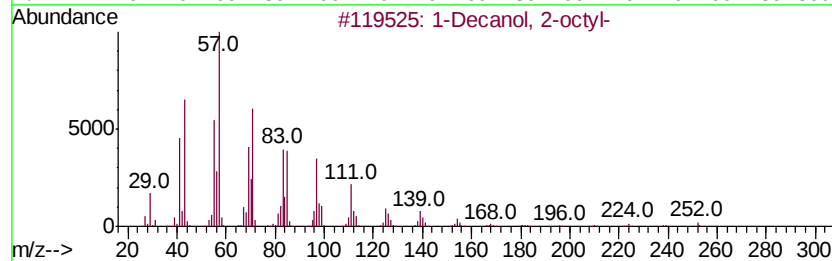
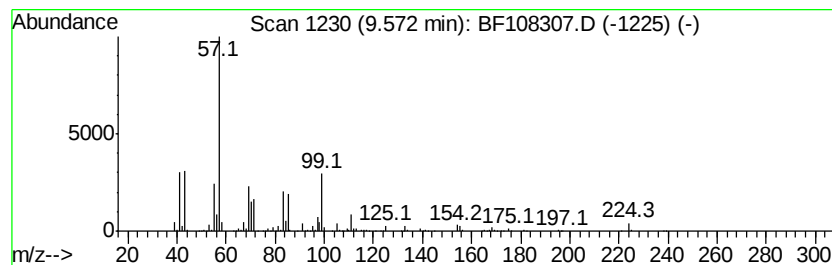
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Decanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	25.13 ng	1472410	Acenaphthene-d10	10.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decanol, 2-octyl-	270 C18H38O	045235-48-1	50
2	2-Azido-2,4,4,6,6,8,8-heptamethy...	267 C16H33N3	1000293-29-1	47
3	1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6	42
4	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	38
5	2-Butenedioic acid (E)-, bis(2-e...	340 C20H36O4	000141-02-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
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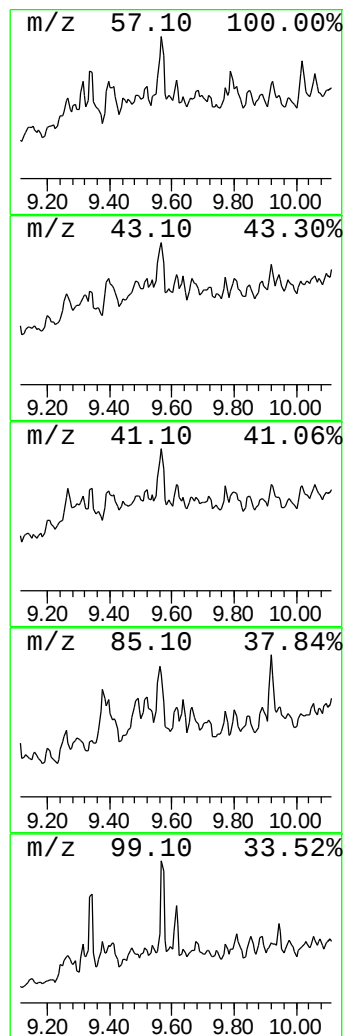
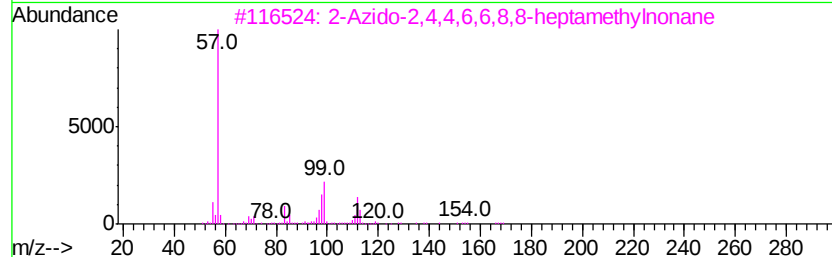
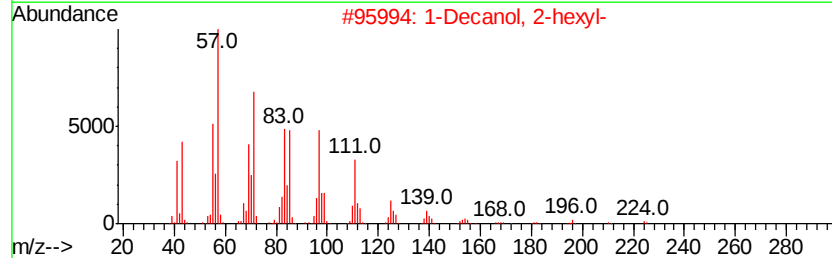
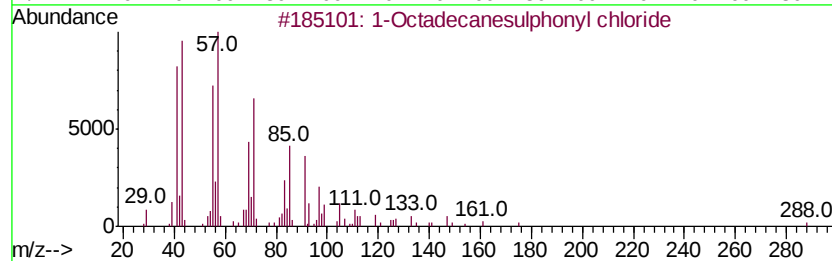
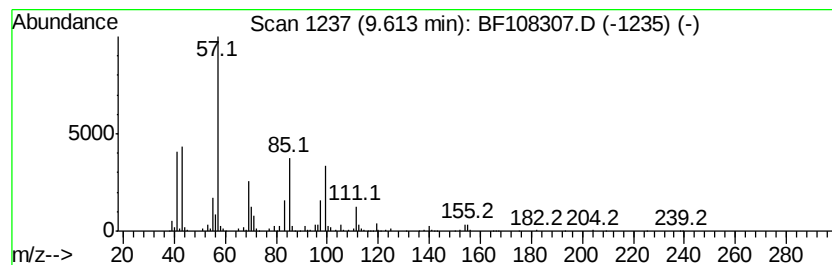
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Octadecanesulphonyl chloride Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	8.07 ng	473069	Acenaphthene-d10	10.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	53
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47
3			2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	47
4			Neopentyl isobutyl ketone	156	C10H20O	040239-19-8	43
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
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Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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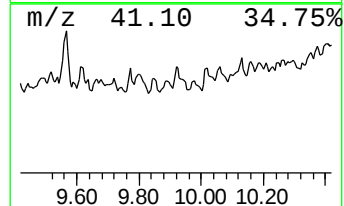
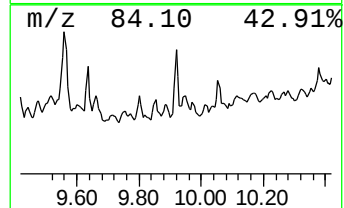
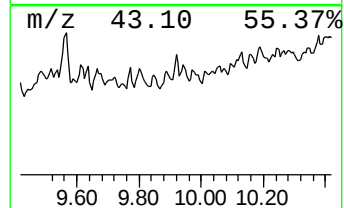
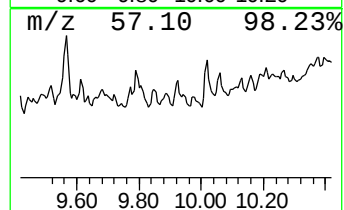
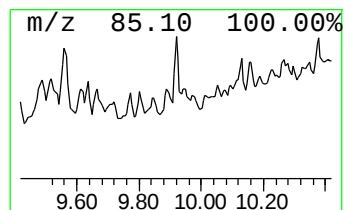
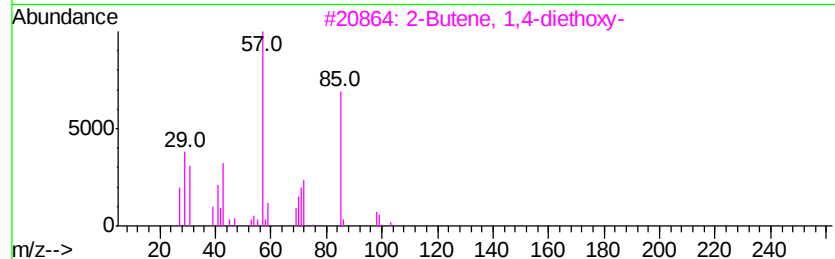
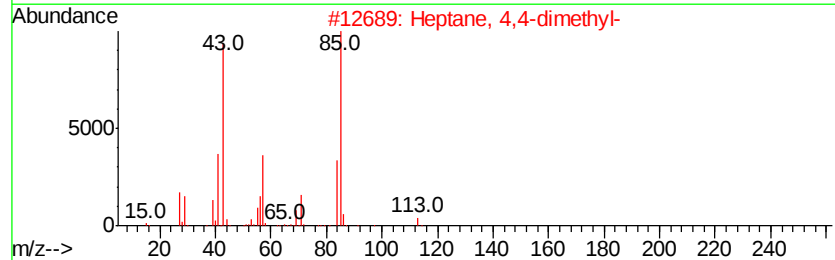
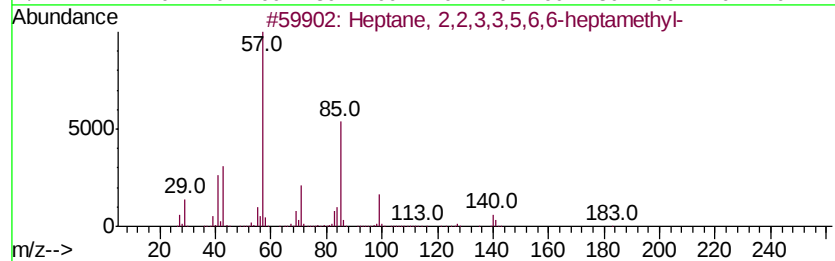
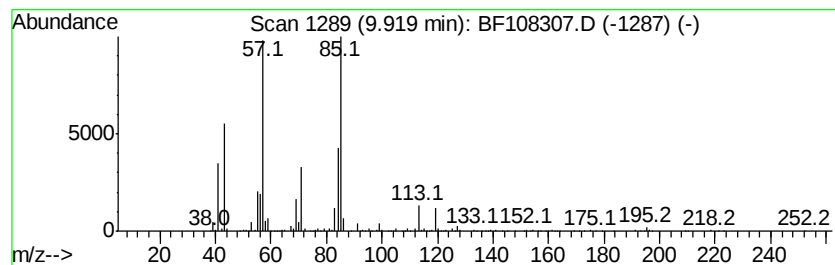
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown9.92 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	11.76 ng	689139	Acenaphthene-d10	10.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	47
2			Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	43
3			2-Butene, 1,4-diethoxy-	144	C8H16O2	007250-85-3	43
4			5-Dodecanone	184	C12H24O	019780-10-0	40
5			3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
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Sample : J4539-02
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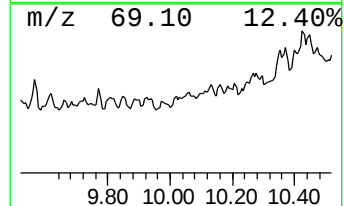
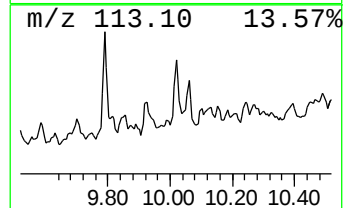
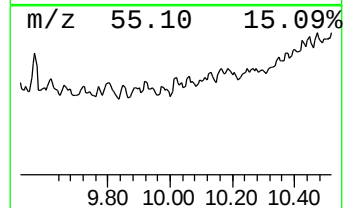
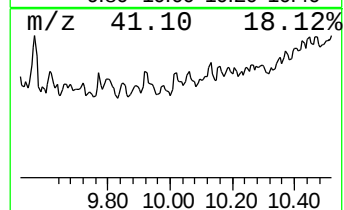
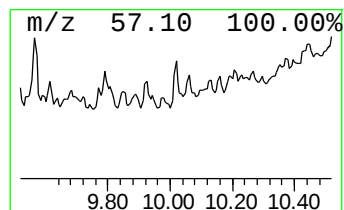
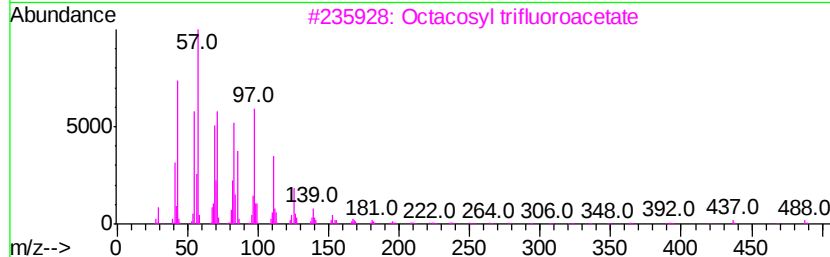
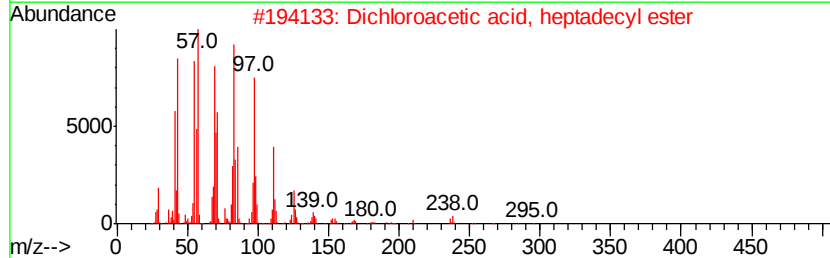
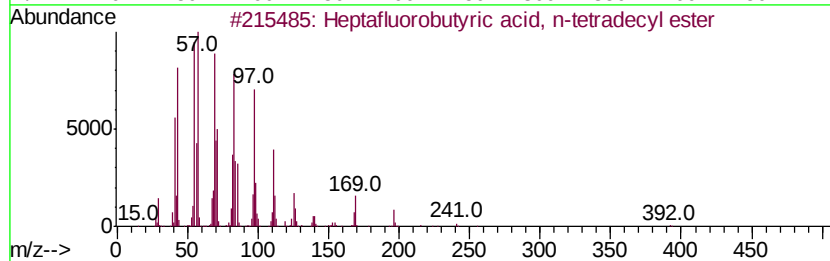
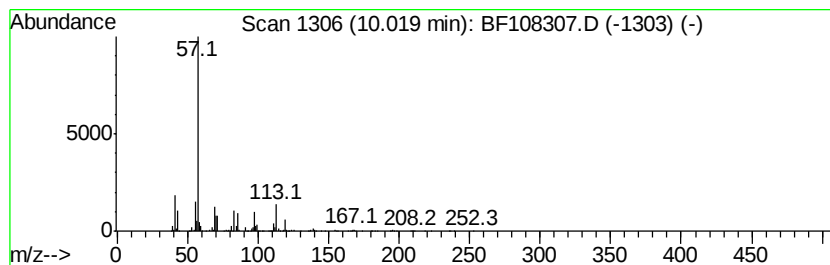
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown10.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	16.99 ng	995803	Acenaphthene-d10	10.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8 47
2		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 47
3		Octacosyl trifluoroacetate	506 C30H57F3O2	1000351-74-9 43
4		1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6 43
5		Heptadecyl heptafluorobutyrate	452 C21H35F7O2	959085-66-6 43



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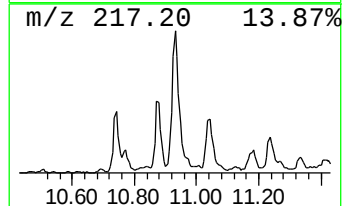
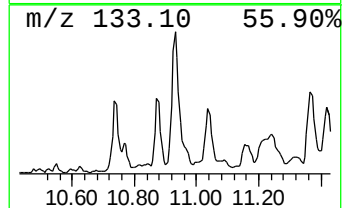
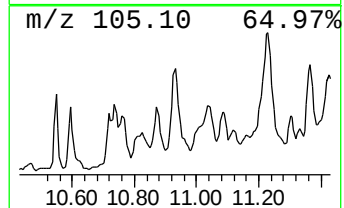
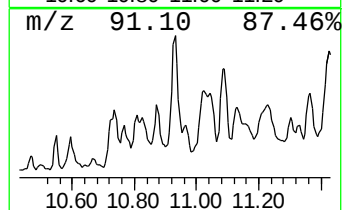
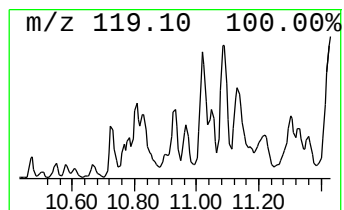
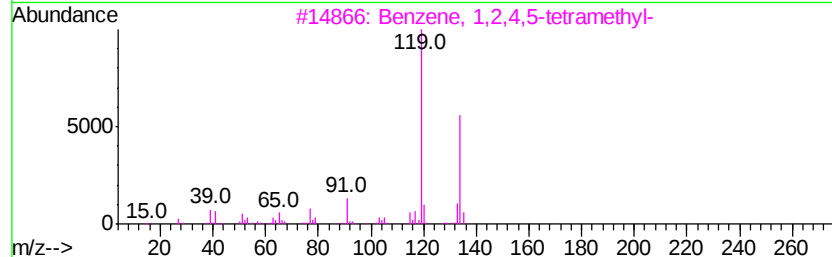
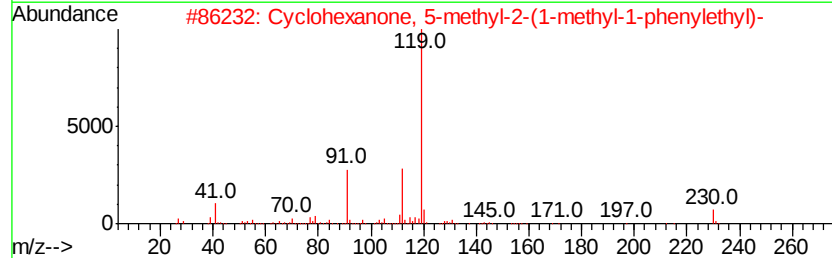
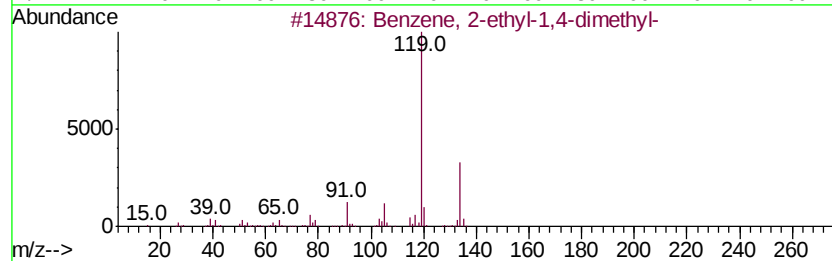
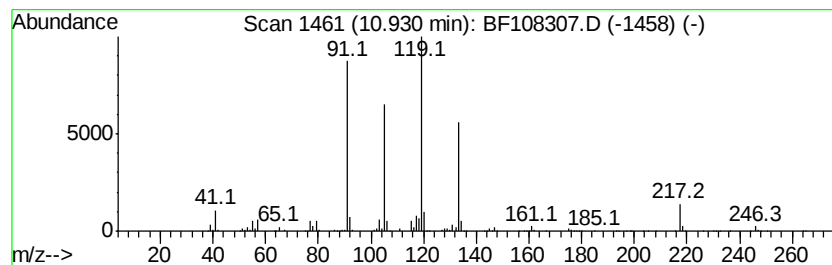
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	10.61 ng	2290980	Phenanthrene-d10	11.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	58
2		Cyclohexanone, 5-methyl-2-(1-met...	230	C16H22O	097275-48-4	50
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	47
4		Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	000140-76-1	47
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
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ClientSampleId :
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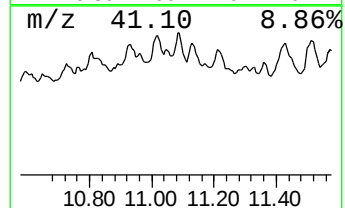
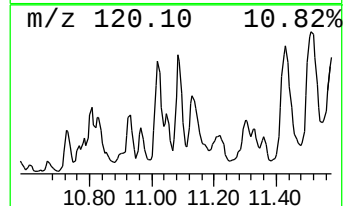
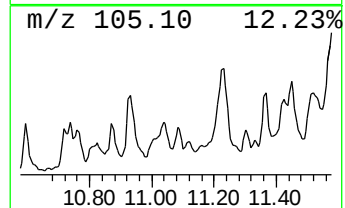
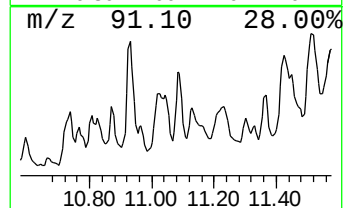
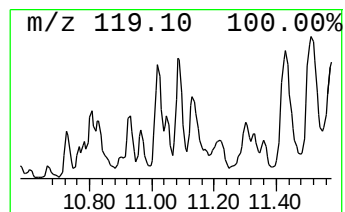
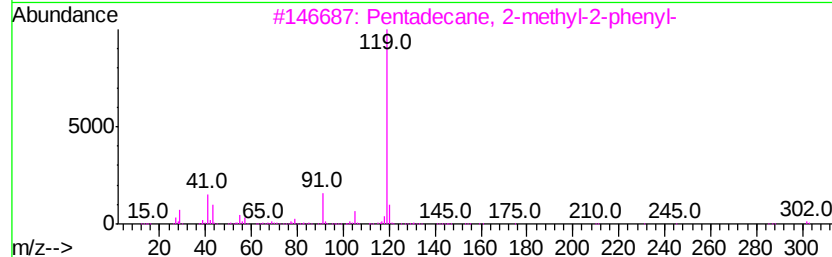
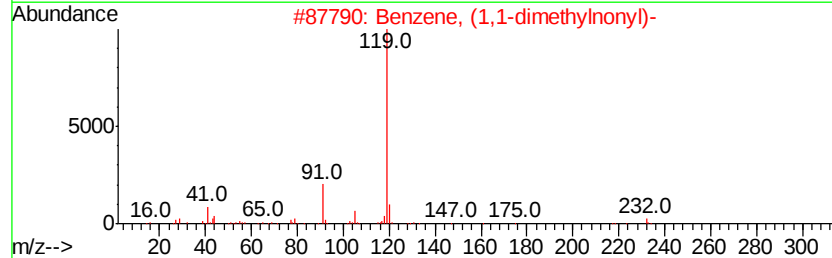
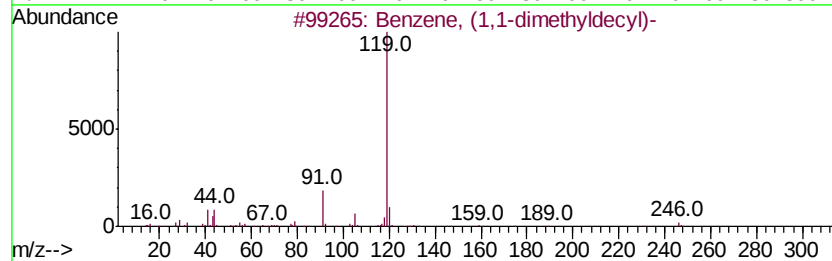
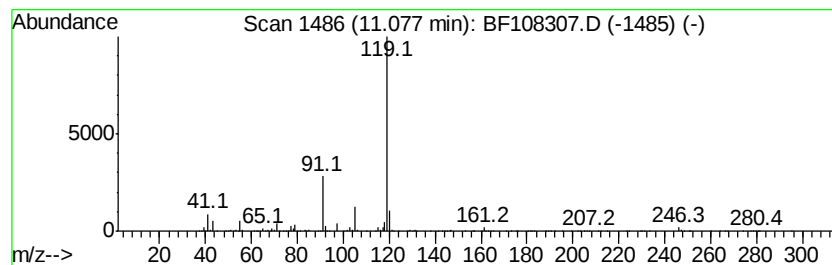
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzene, (1,1-dimethyldecyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	12.03 ng	2596370	Phenanthrene-d10	11.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	91
2		Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	78
3		Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	78
4		Dicumyl peroxide	270	C18H22O2	000080-43-3	72
5		[5-(4-Ethylphenyl)-5-hydroxy-3-t...	376	C20H19F3N2O2	1000311-59-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108307.D
Acq On : 20 Aug 2018 23:00
Operator : JU/SJ
Sample : J4539-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MS-RO-27186

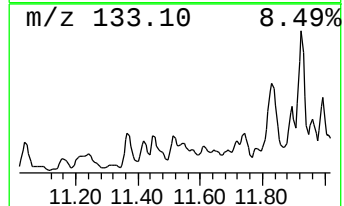
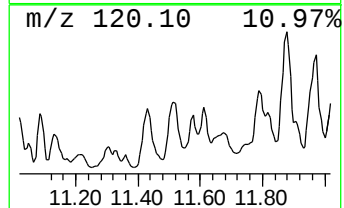
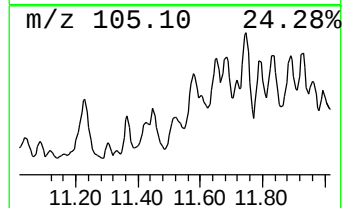
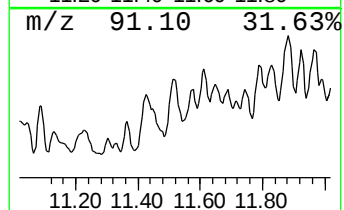
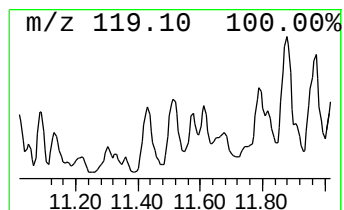
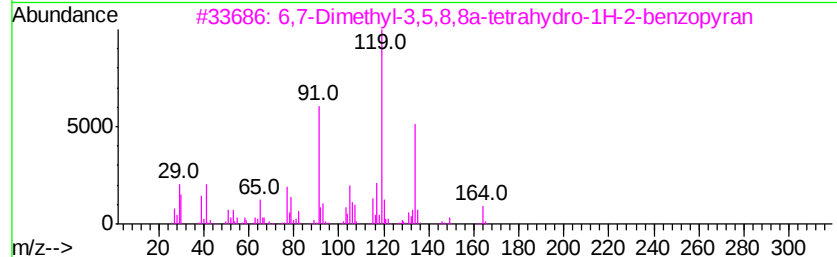
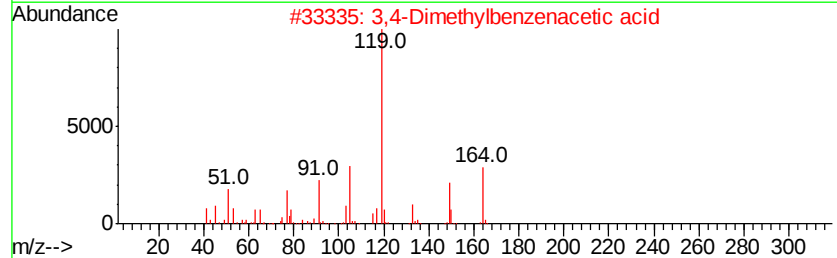
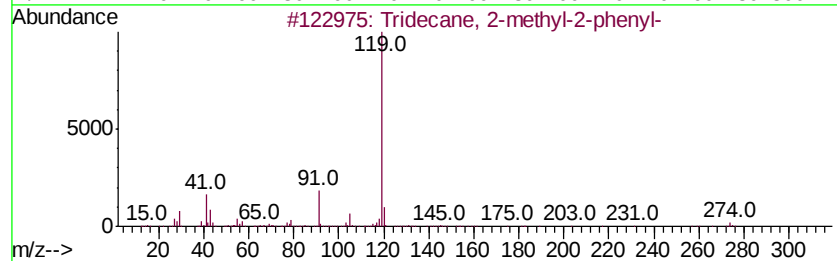
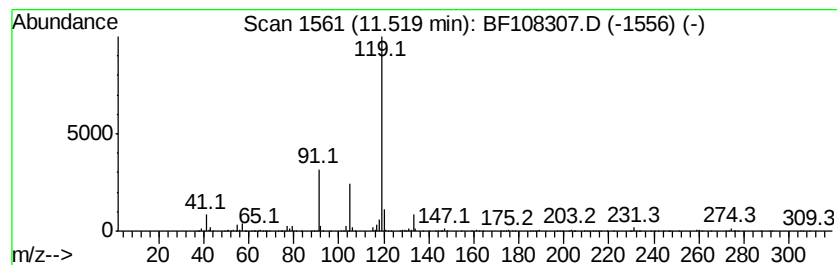
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Tridecane, 2-methyl-2-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	20.00 ng	4317430	Phenanthrene-d10	11.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	74
2		3,4-Dimethylbenzenacetic acid	164	C10H12O2	017283-16-8	72
3		6,7-Dimethyl-3,5,8,8a-tetrahydro...	164	C11H16O	110028-10-9	72
4		Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	59
5		[5-(4-Ethylphenyl)-5-hydroxy-3-t...	376	C20H19F3N2O2	1000311-59-5	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082018\
 Data File : BF108307.D
 Acq On : 20 Aug 2018 23:00
 Operator : JU/SJ
 Sample : J4539-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MS-RO-27186

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	2.37	10.3	ng	482019	1	7.02	937758	20.0
unknown6.79	6.79	74.8	ng	3508870	1	7.02	937758	20.0
unknown6.82	6.82	5.3	ng	247314	1	7.02	937758	20.0
7-Oxabicyclo[4.1....	8.67	5.0	ng	280017	2	8.30	1116470	20.0
Cyclopentanecarbo...	8.80	8.3	ng	461907	2	8.30	1116470	20.0
unknown8.86	8.86	9.8	ng	549185	2	8.30	1116470	20.0
Sulfurous acid, b...	8.90	5.2	ng	290913	2	8.30	1116470	20.0
unknown8.97	8.97	11.2	ng	625847	2	8.30	1116470	20.0
unknown9.02	9.02	10.2	ng	568563	2	8.30	1116470	20.0
unknown9.05	9.05	7.1	ng	395261	2	8.30	1116470	20.0
4-Heptanol, 2,6-d...	9.20	9.0	ng	527271	3	10.07	1171940	20.0
Sulfurous acid, c...	9.27	17.6	ng	1032180	3	10.07	1171940	20.0
1-Decanol, 2-octyl-	9.57	25.1	ng	1472410	3	10.07	1171940	20.0
1-Octadecanesulph...	9.61	8.1	ng	473069	3	10.07	1171940	20.0
unknown9.92	9.92	11.8	ng	689139	3	10.07	1171940	20.0
unknown10.02	10.02	17.0	ng	995803	3	10.07	1171940	20.0
Benzene, 2-ethyl-...	10.93	10.6	ng	2290980	4	11.58	4317430	20.0
Benzene, (1,1-dim...	11.08	12.0	ng	2596370	4	11.58	4317430	20.0
Tridecane, 2-meth...	11.52	20.0	ng	4317430	4	11.58	4317430	20.0