

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
 Data File : BF102157.D
 Acq On : 17 Jan 2018 18:33
 Operator : SJ/JU
 Sample : J1152-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LTP-4

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-BF010918.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	4.928	477	483	491	rVB	155298	223382	7.45%	0.907%
2	5.334	546	552	555	rBV	3005652	2934655	97.92%	11.922%
3	6.357	721	726	730	rBV	2742458	2984894	99.59%	12.126%
4	6.492	744	749	752	rBV	3037121	2997122	100.00%	12.176%
5	6.722	784	788	791	rBV	943934	751684	25.08%	3.054%
6	6.875	810	814	817	rBV	2565867	2232543	74.49%	9.070%
7	7.286	878	884	887	rBV	1995016	1808279	60.33%	7.346%
8	7.998	1002	1005	1009	rBV	1103343	945442	31.54%	3.841%
9	8.557	1097	1100	1104	rBV	167007	131787	4.40%	0.535%
10	9.080	1184	1189	1192	rBV	3110953	2733517	91.20%	11.105%
11	9.469	1252	1255	1259	rBV	326967	267906	8.94%	1.088%
12	9.751	1299	1303	1307	rBV2	999863	859356	28.67%	3.491%
13	10.463	1421	1424	1428	rBV	423518	376721	12.57%	1.530%
14	10.539	1433	1437	1440	rBV	1574382	1327025	44.28%	5.391%
15	11.233	1551	1555	1559	rBV	794843	633583	21.14%	2.574%
16	12.815	1820	1824	1828	rBV	1643861	1559620	52.04%	6.336%
17	13.709	1973	1976	1985	rBV	92333	102048	3.40%	0.415%
18	13.862	1998	2002	2006	rBV	718281	645521	21.54%	2.622%
19	14.615	2127	2130	2137	rVB	169008	185202	6.18%	0.752%
20	14.774	2154	2157	2162	rVB4	35584	35136	1.17%	0.143%
21	14.980	2189	2192	2198	rVB5	39682	47101	1.57%	0.191%
22	15.280	2238	2243	2253	rBV	602764	730685	24.38%	2.968%
23	15.721	2314	2318	2322	rBV	37222	51443	1.72%	0.209%
24	17.198	2563	2569	2576	rBV	24232	50650	1.69%	0.206%

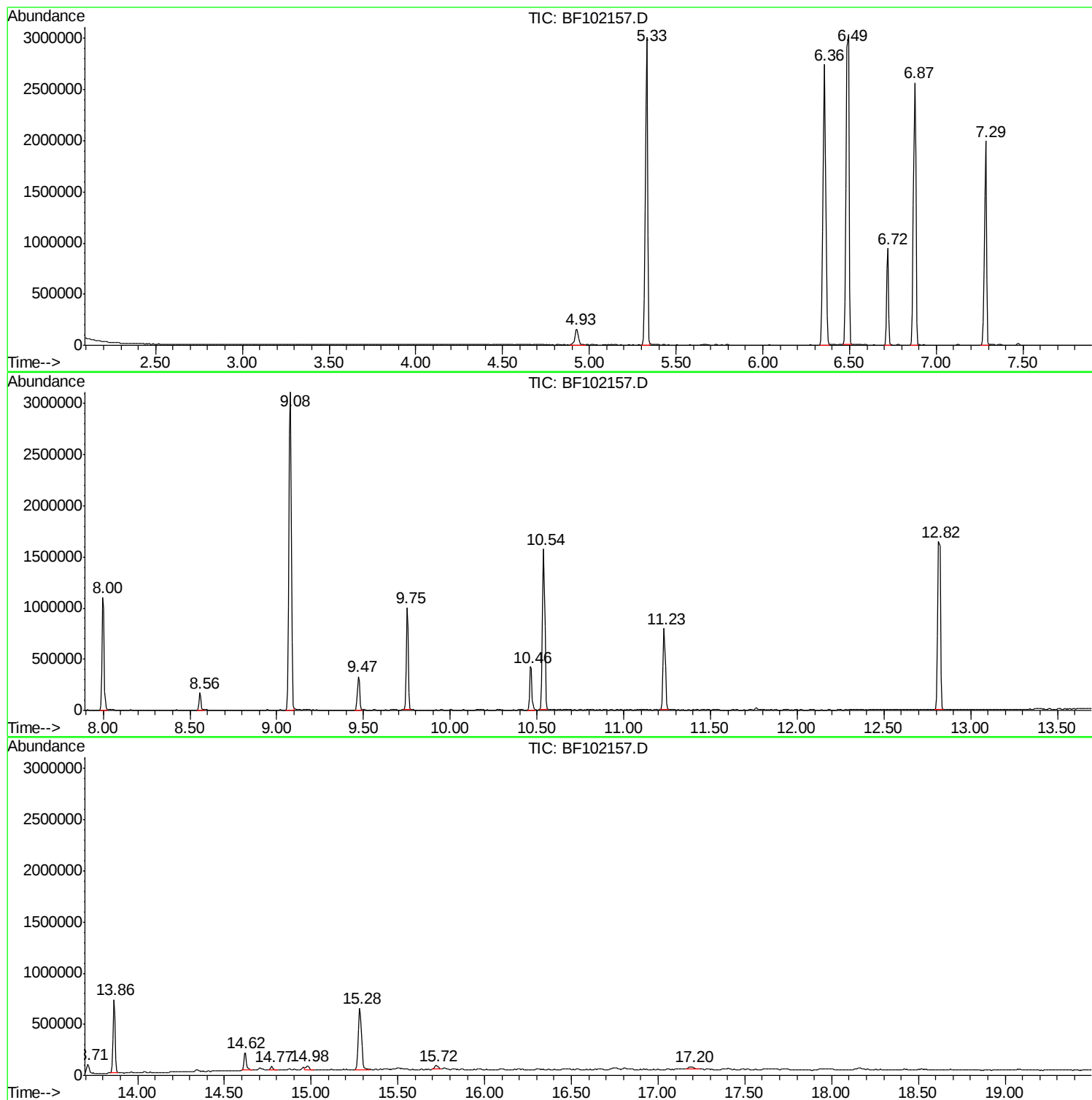
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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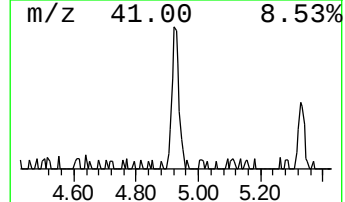
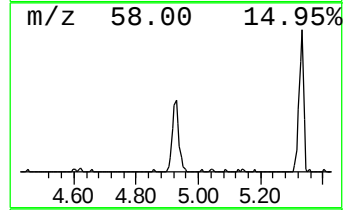
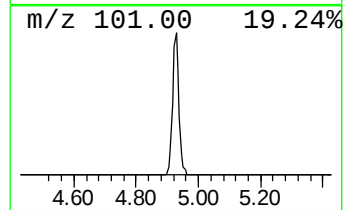
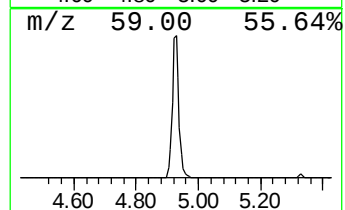
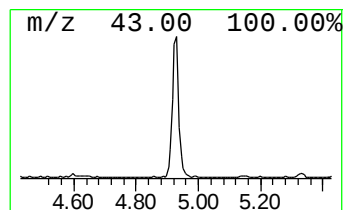
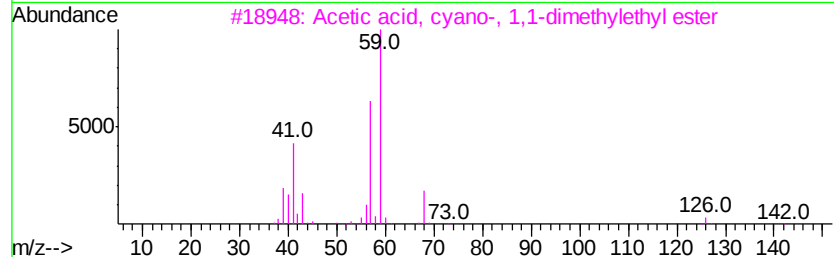
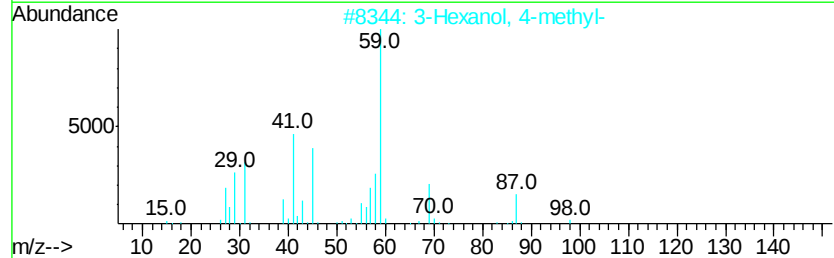
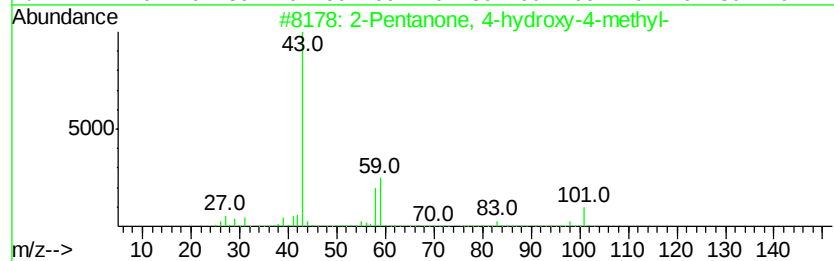
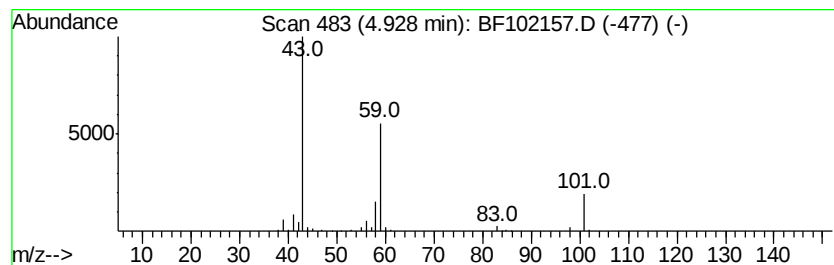
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.93	5.94 ng	223382	1,4-Dichlorobenzene-d4	6.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Silane, dimethyl-	60	C2H8Si	001111-74-6	9



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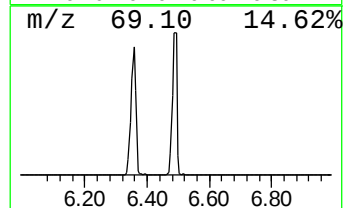
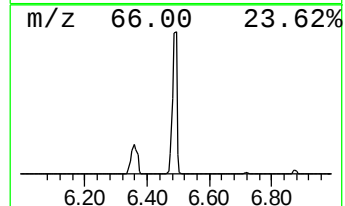
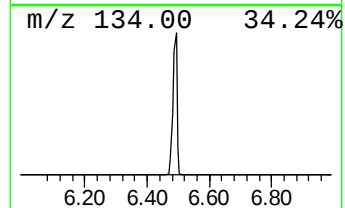
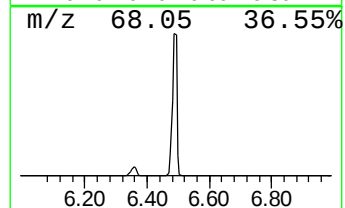
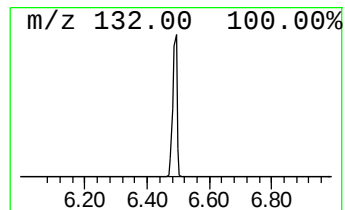
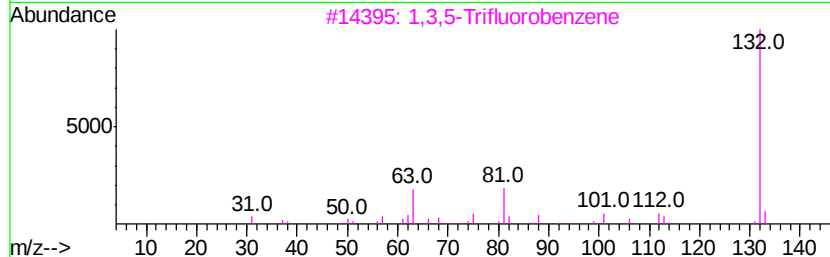
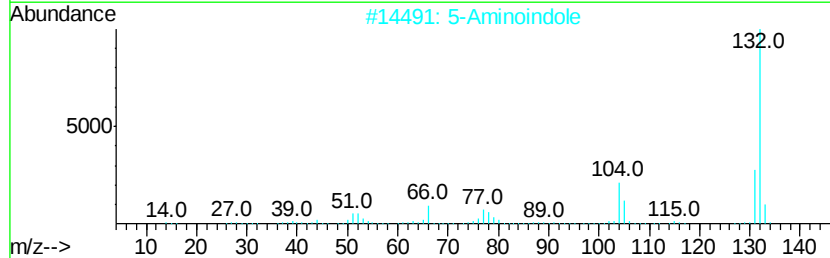
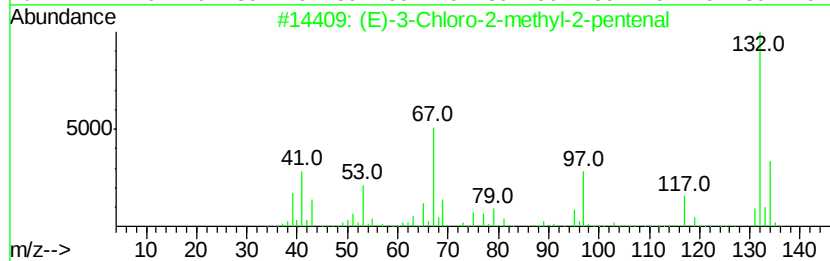
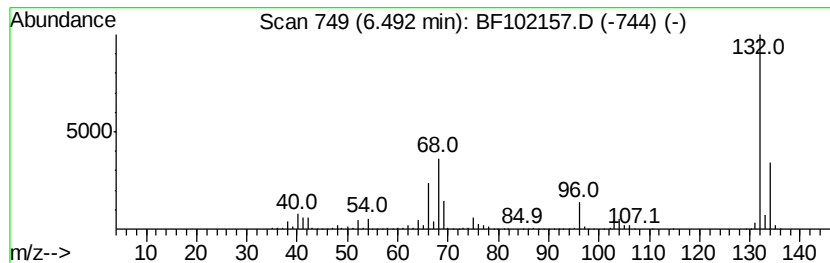
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	79.74 ng	2997120	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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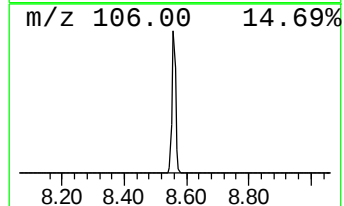
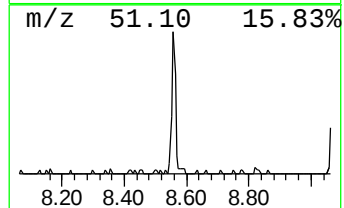
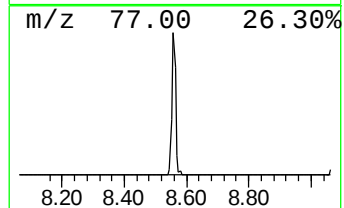
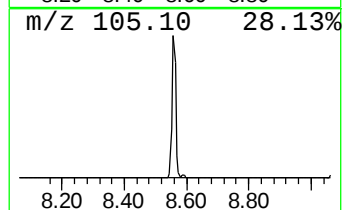
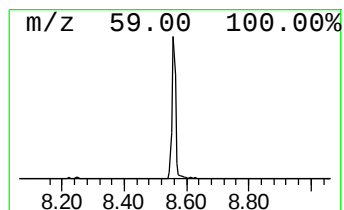
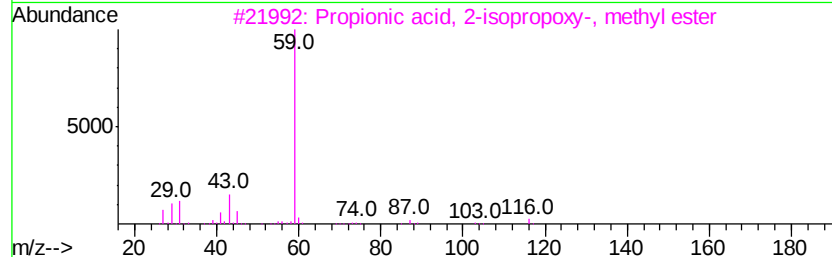
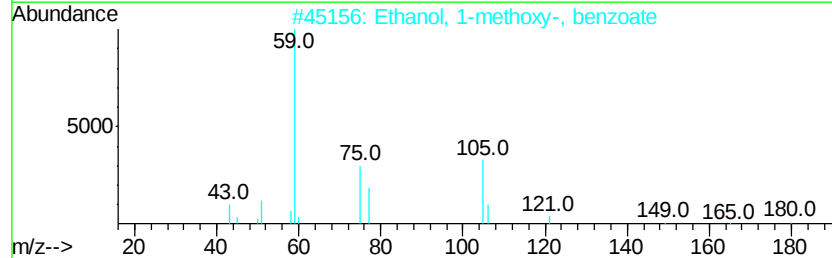
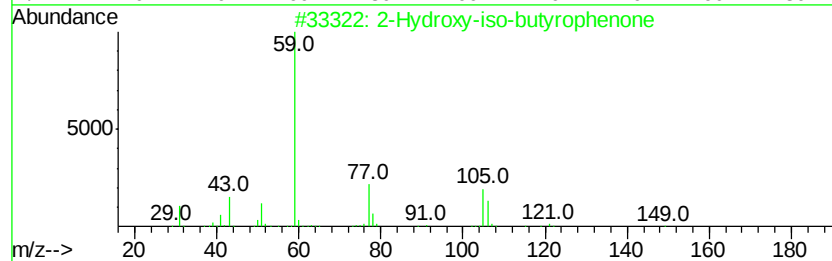
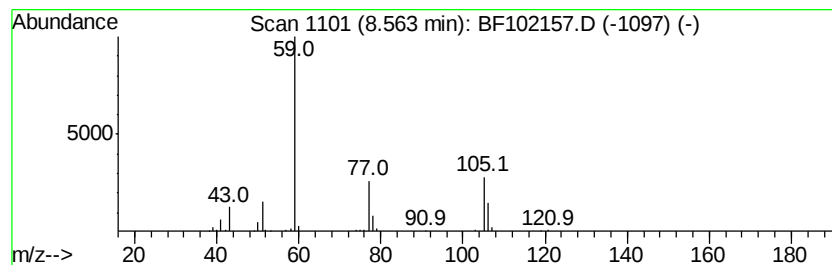
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	2.79 ng	131787	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



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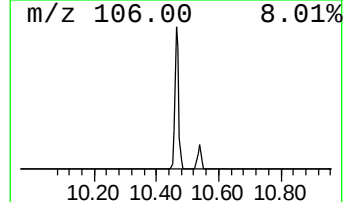
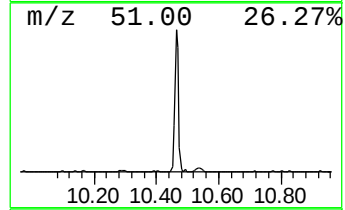
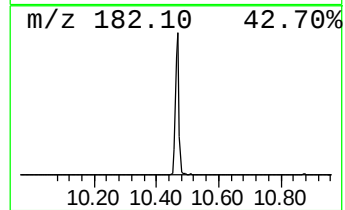
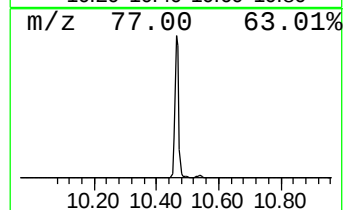
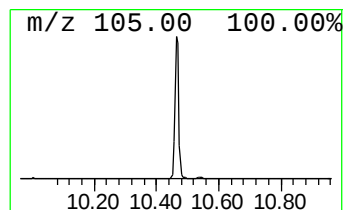
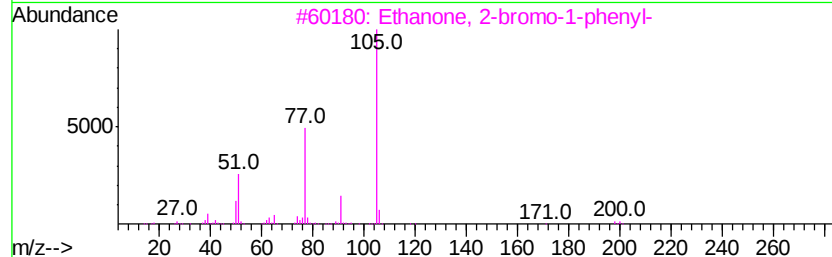
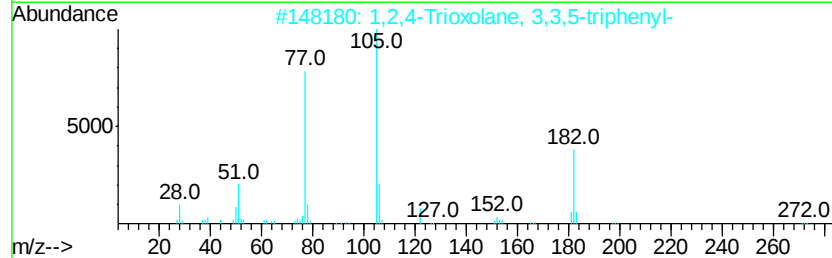
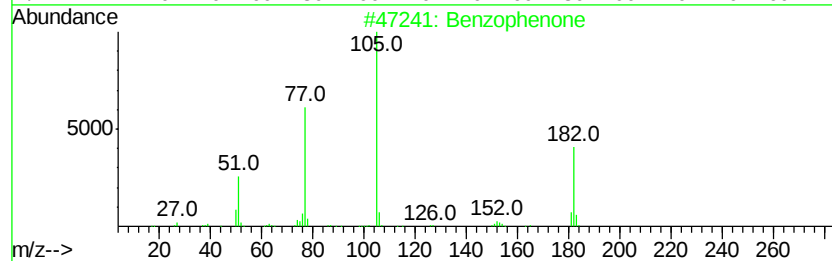
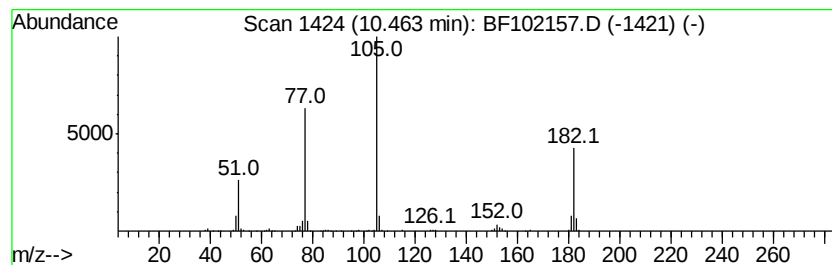
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	8.77 ng	376721	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3		Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47
4		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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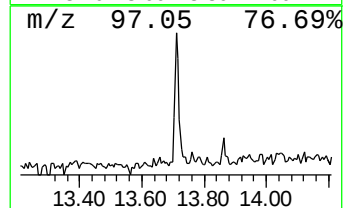
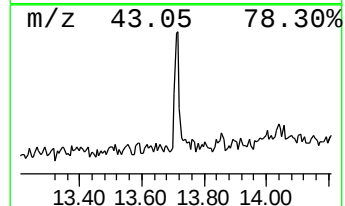
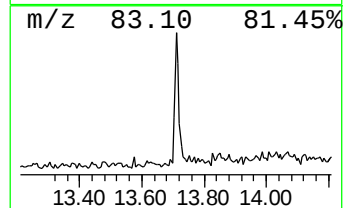
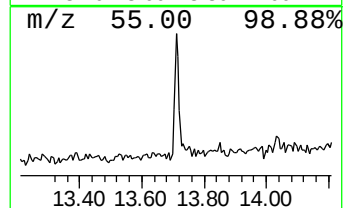
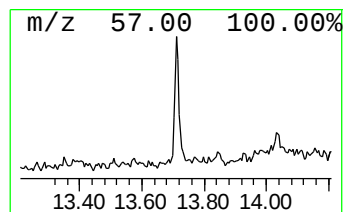
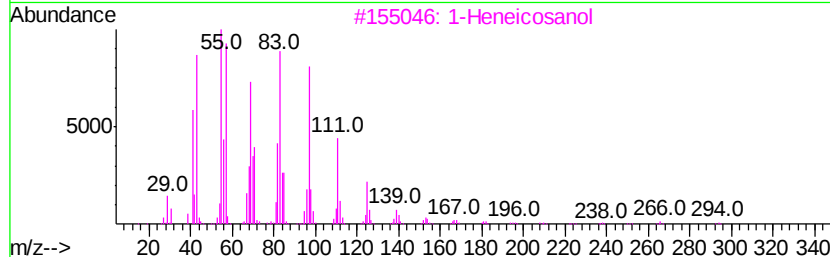
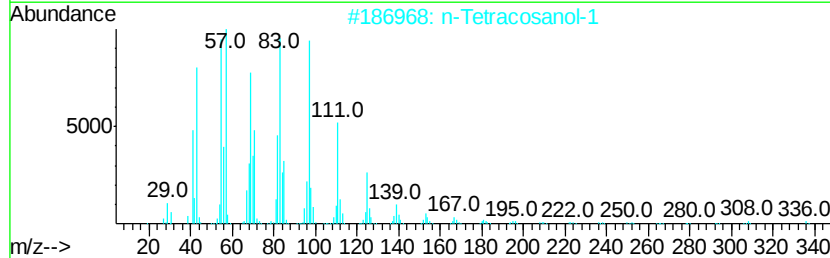
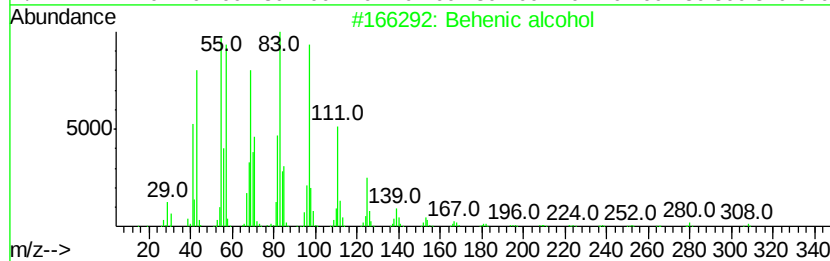
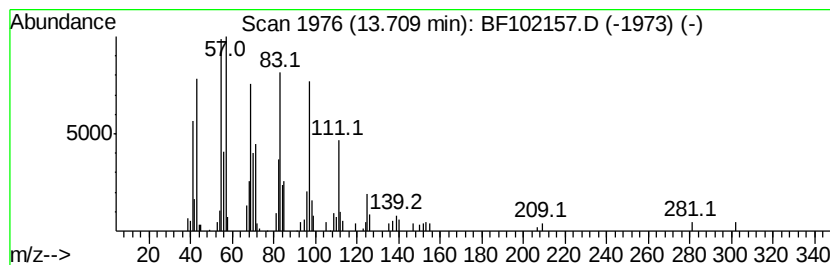
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Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	3.16 ng	102048	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Octacosanol	410	C28H58O	000557-61-9	93
5	1-Nonadecene	266	C19H38	018435-45-5	91



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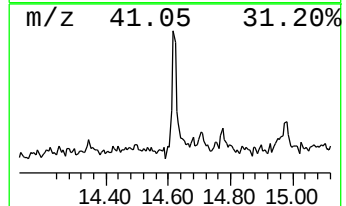
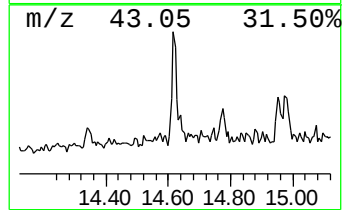
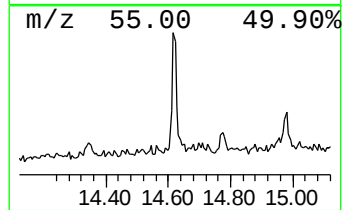
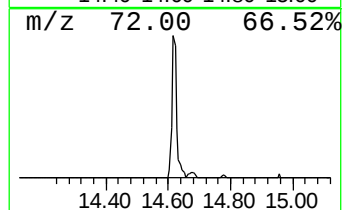
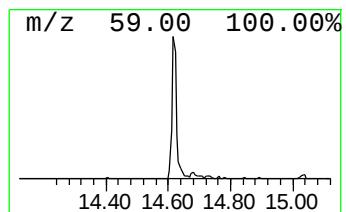
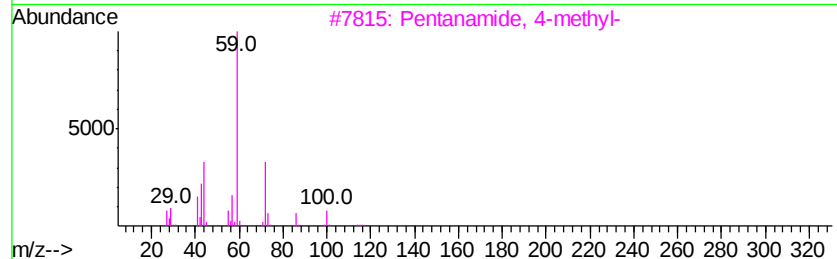
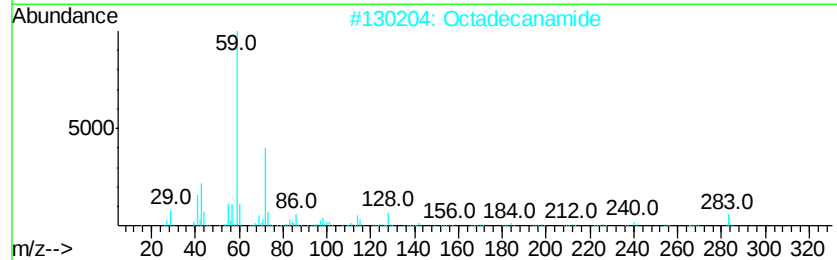
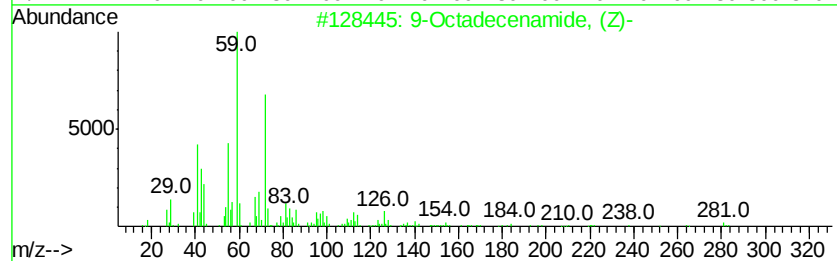
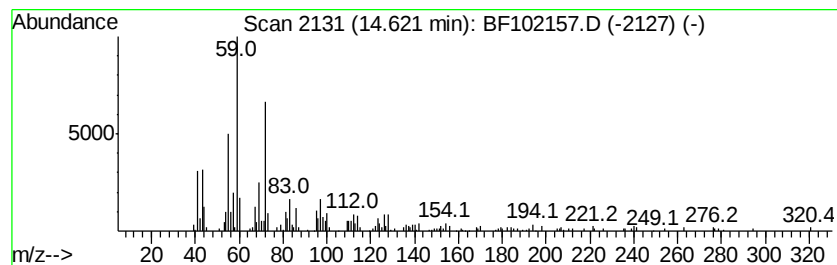
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.07 ng	185202	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2		Octadecanamide	283	C18H37NO	000124-26-5	72
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4		Hexadecanamide	255	C16H33NO	000629-54-9	53
5		3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	47



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
Data File : BF102157.D
Acq On : 17 Jan 2018 18:33
Operator : SJ/JU
Sample : J1152-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LTP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.93	5.9	ng	223382	1	6.72	751684	20.0
unknown6.49	6.49	79.7	ng	2997120	1	6.72	751684	20.0
2-Hydroxy-iso-but...	8.56	2.8	ng	131787	2	8.00	945442	20.0
Benzophenone	10.46	8.8	ng	376721	3	9.75	859356	20.0
Behenic alcohol	13.71	3.2	ng	102048	5	13.86	645521	20.0
9-Octadecenamide, ...	14.62	5.1	ng	185202	6	15.28	730685	20.0