

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
 Data File : BF109717.D
 Acq On : 10 Oct 2018 1:36
 Operator : JU/SJ
 Sample : J5329-05
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 POND-2

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-BF100818.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	4.898	475	478	494	rBV	39324	62757	3.21%	0.388%
2	5.316	545	549	579	rBV	1272282	1596350	81.57%	9.874%
3	6.345	720	724	741	rBV	1290215	1723290	88.05%	10.659%
4	6.469	741	745	770	rVB	1641273	1906289	97.40%	11.791%
5	6.698	780	784	806	rVB	299003	456292	23.31%	2.822%
6	6.851	806	810	835	rBV	1389437	1392147	71.13%	8.611%
7	7.257	876	879	906	rBV	765323	1145334	58.52%	7.084%
8	7.975	998	1001	1032	rBV	418109	567684	29.01%	3.511%
9	9.051	1180	1184	1202	rBV	1818097	1957137	100.00%	12.105%
10	9.445	1247	1251	1262	rBV	161962	174311	8.91%	1.078%
11	9.722	1294	1298	1313	rBV	557631	553168	28.26%	3.421%
12	10.510	1428	1432	1451	rBV	736941	962632	49.19%	5.954%
13	11.198	1546	1549	1566	rBV	346013	489495	25.01%	3.028%
14	11.739	1638	1641	1649	rBV	22806	33524	1.71%	0.207%
15	12.780	1814	1818	1830	rBV	1529306	1556493	79.53%	9.627%
16	13.692	1967	1973	1987	rBV3	58368	161596	8.26%	1.000%
17	13.827	1992	1996	2008	rVB	489904	560312	28.63%	3.466%
18	14.298	2069	2076	2079	rBV2	24844	27801	1.42%	0.172%
19	14.592	2120	2126	2130	rBV	45727	50024	2.56%	0.309%
20	14.662	2134	2138	2142	rVV	39882	39759	2.03%	0.246%
21	14.904	2175	2179	2184	rVB	51487	54269	2.77%	0.336%
22	15.221	2229	2233	2246	rBV	311387	523904	26.77%	3.240%
23	15.645	2300	2305	2314	rVB	50075	75222	3.84%	0.465%
24	16.104	2377	2383	2392	rBV2	33728	66856	3.42%	0.414%
25	16.633	2467	2473	2480	rBV4	16305	30798	1.57%	0.190%

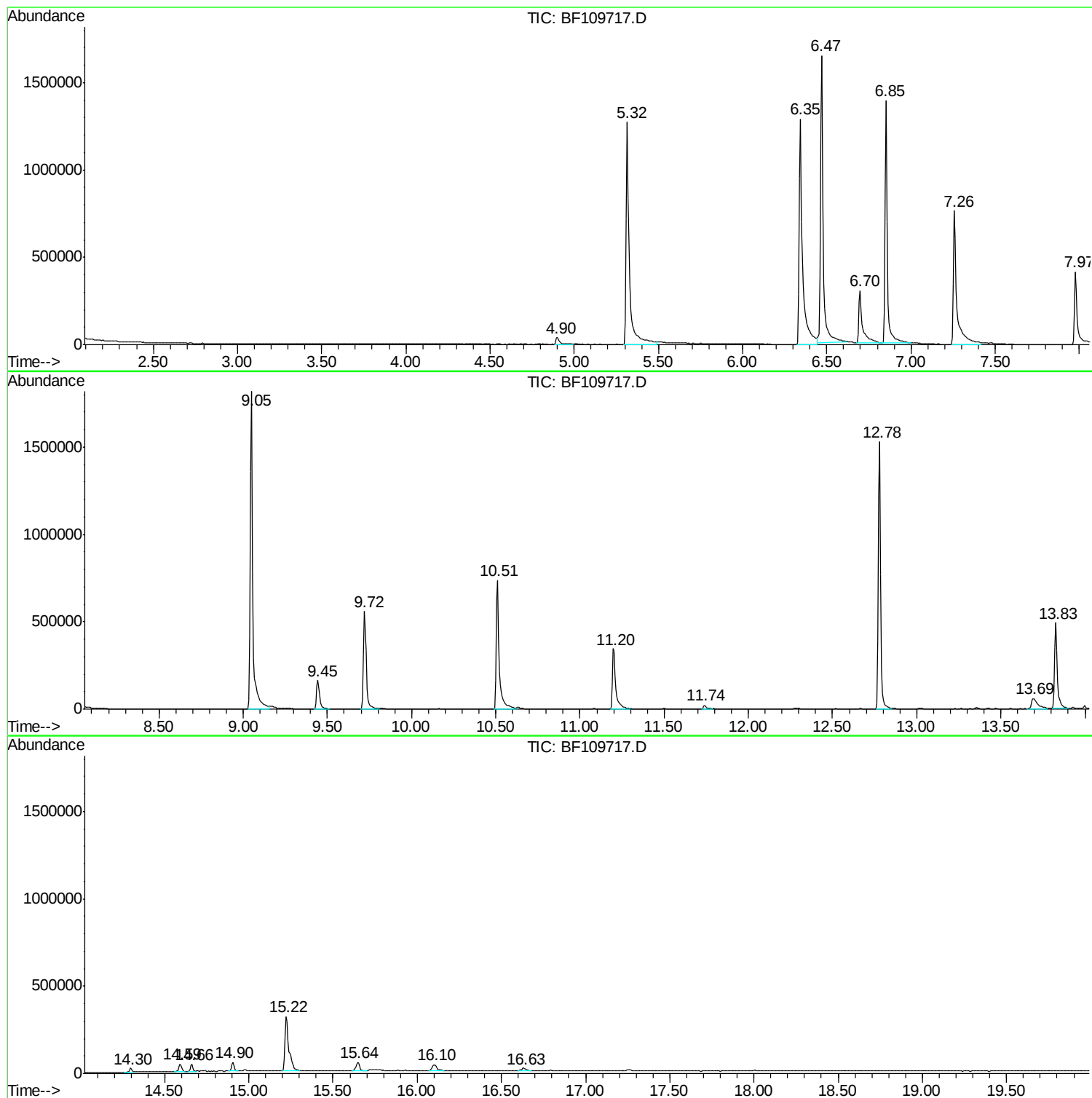
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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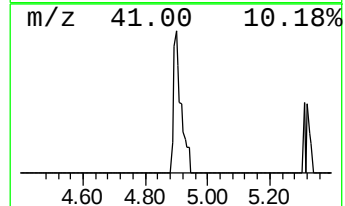
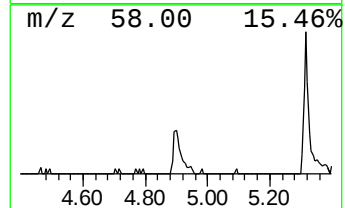
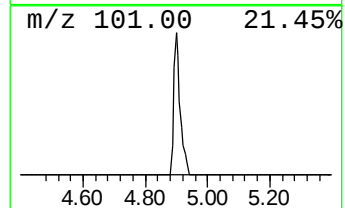
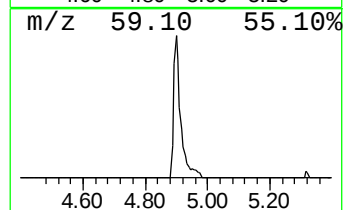
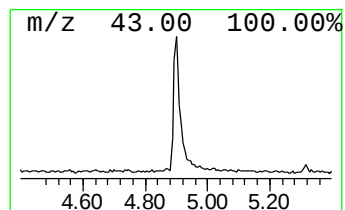
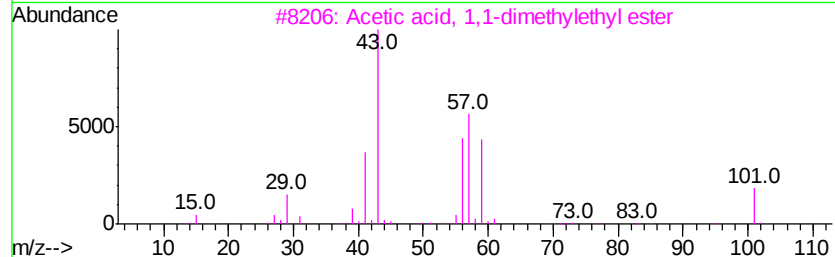
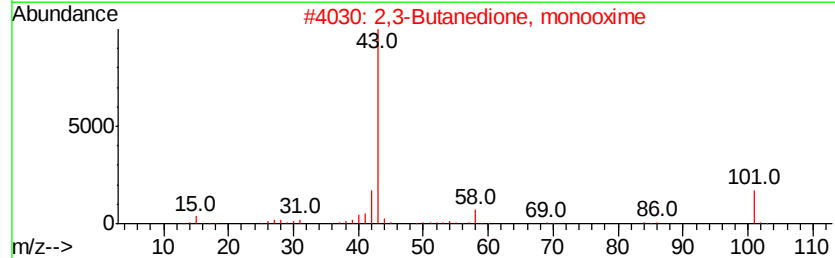
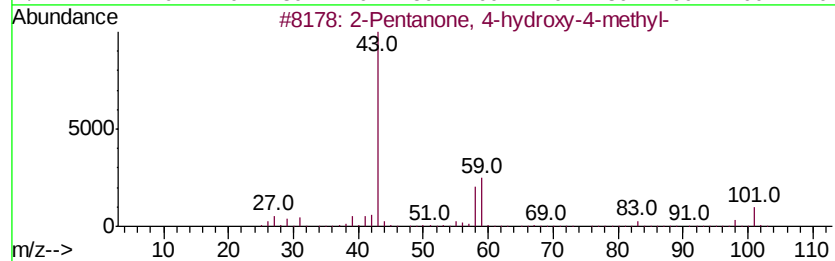
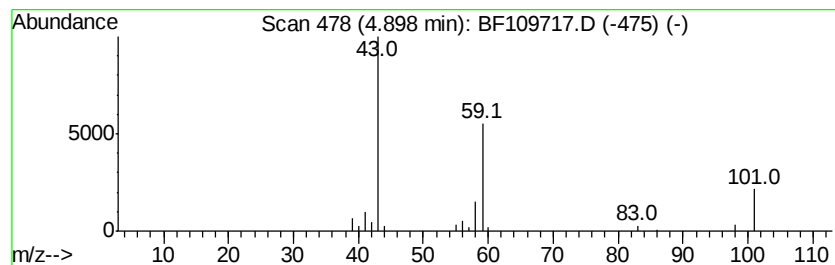
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.90	2.75 ng	62757	1,4-Dichlorobenzene-d4	6.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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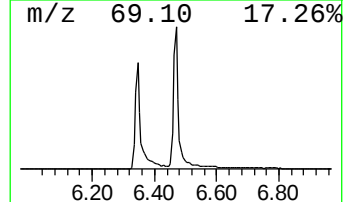
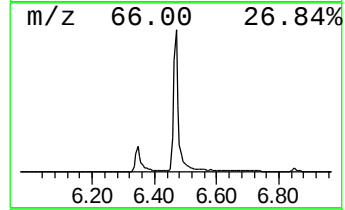
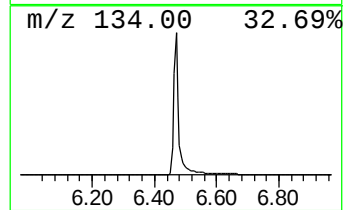
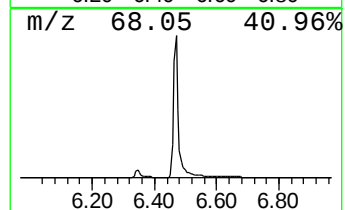
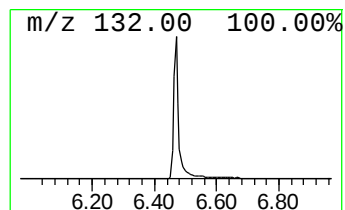
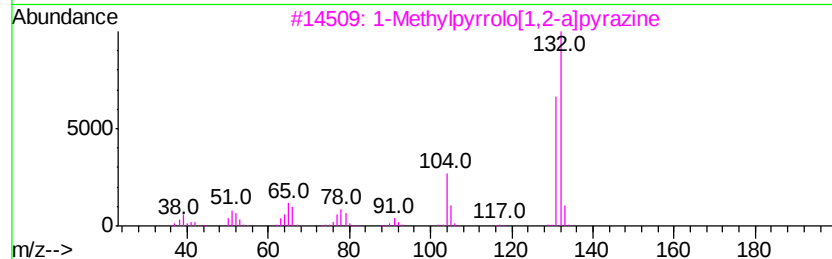
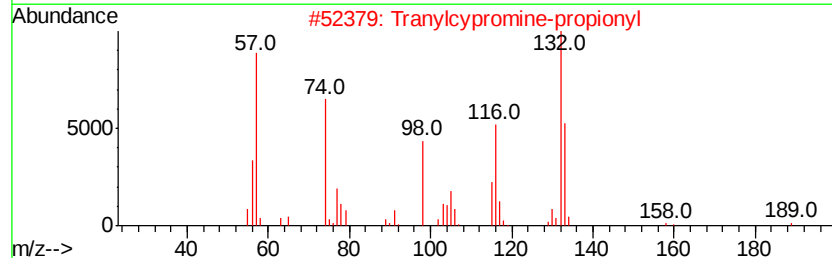
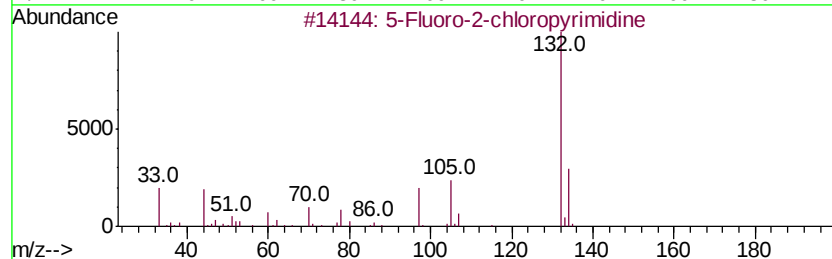
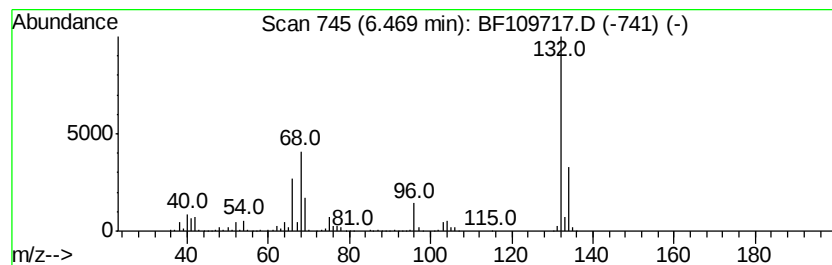
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	83.56 ng	1906290	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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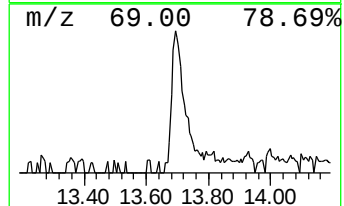
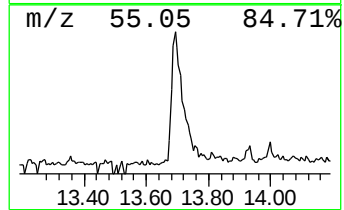
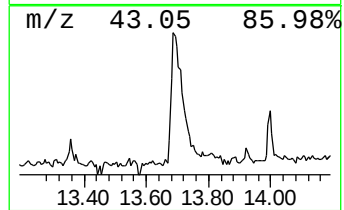
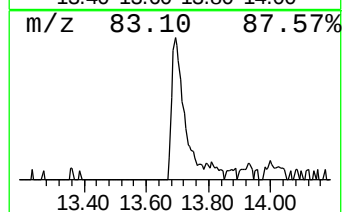
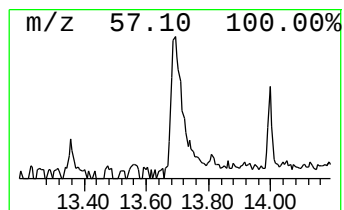
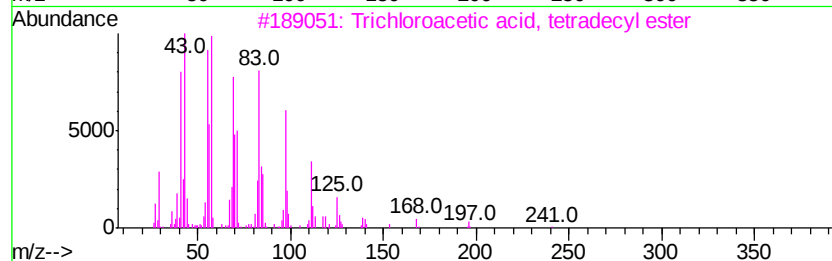
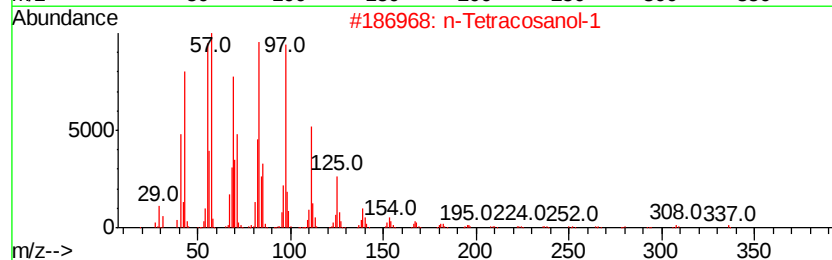
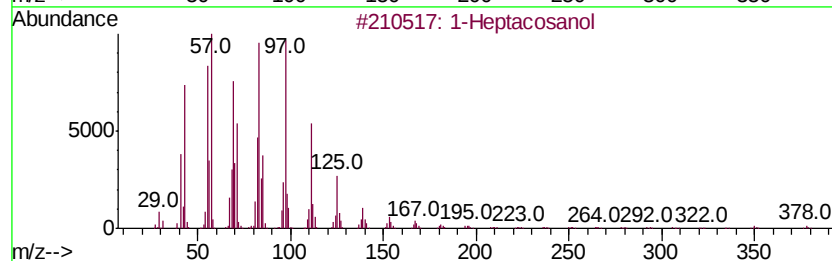
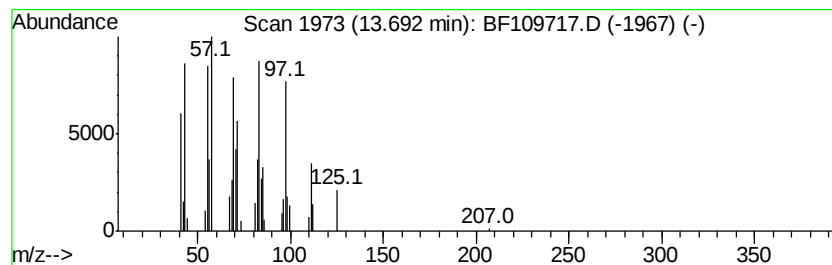
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.69	5.77 ng	161596	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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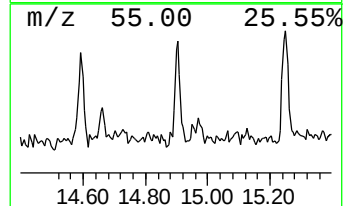
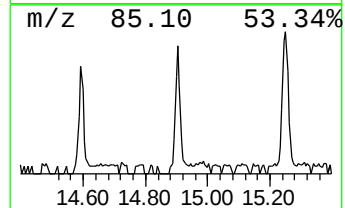
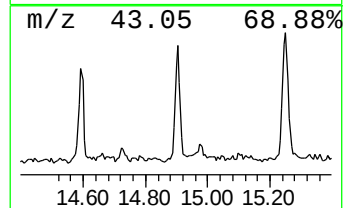
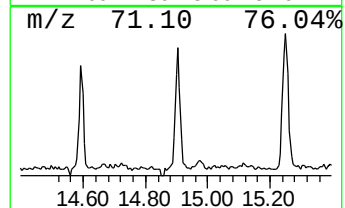
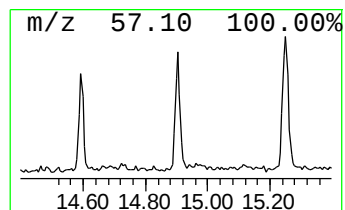
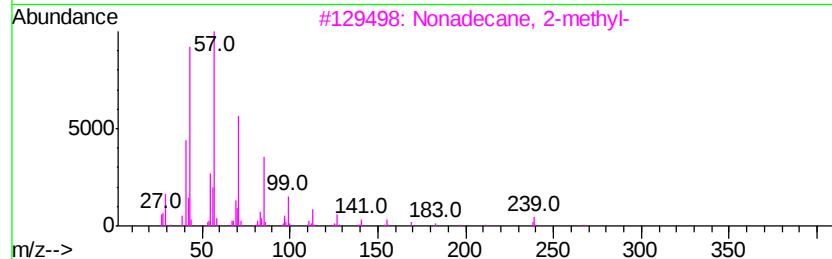
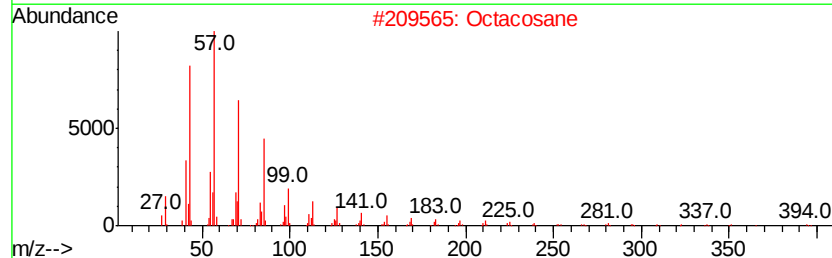
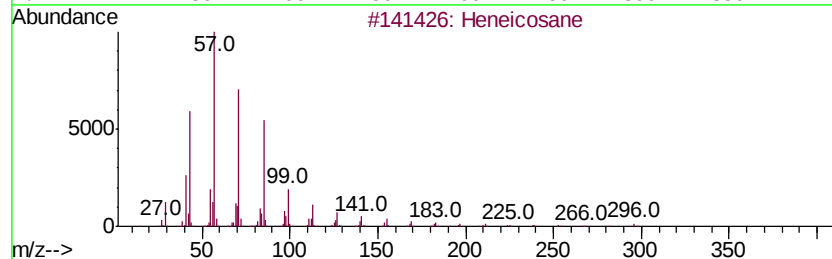
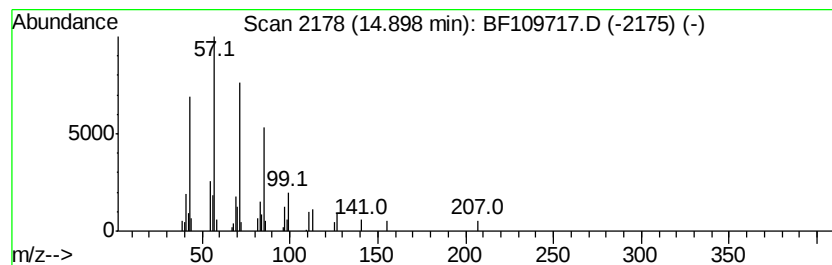
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Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.07 ng	54269	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Nonadecane, 2-methyl-	282 C20H42	001560-86-7	90
4	10-Methylnonadecane	282 C20H42	056862-62-5	87
5	Hexacosane	366 C26H54	000630-01-3	87



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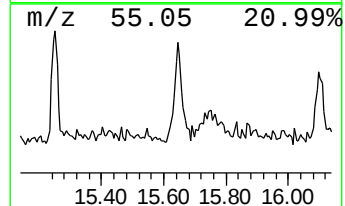
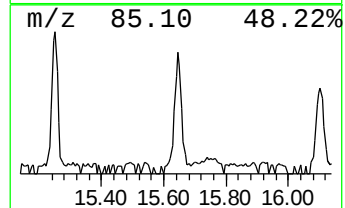
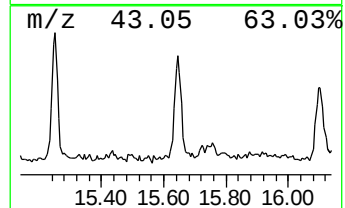
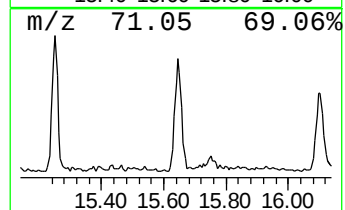
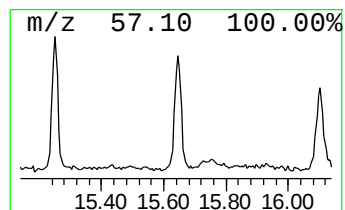
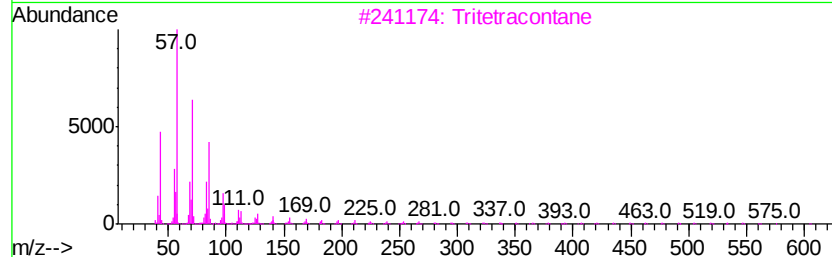
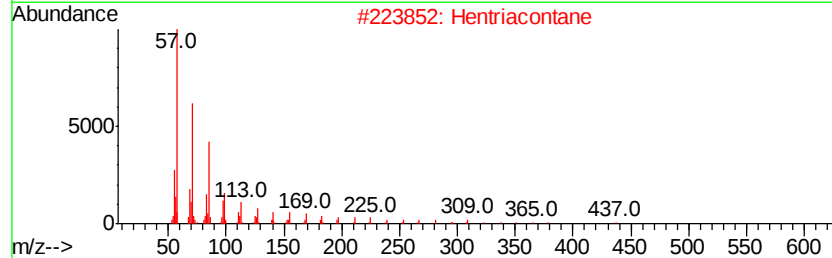
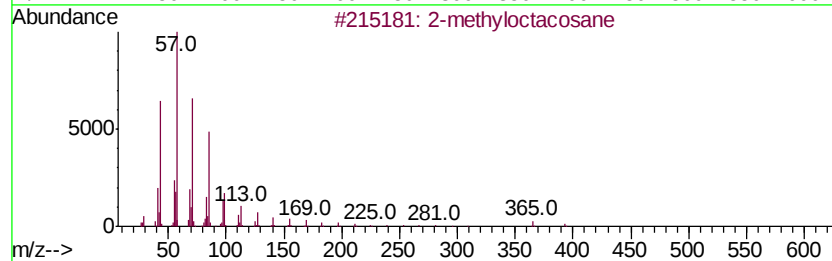
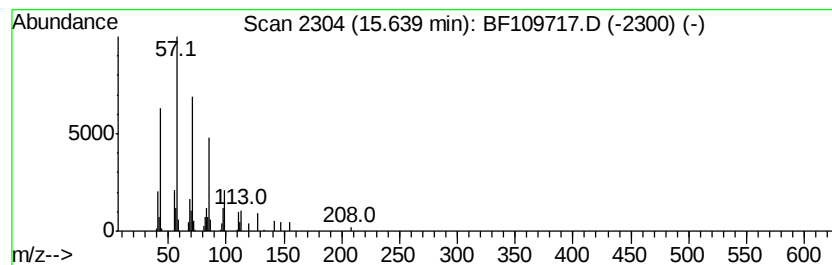
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.87 ng	75222	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Tritetracontane	605	C43H88	007098-21-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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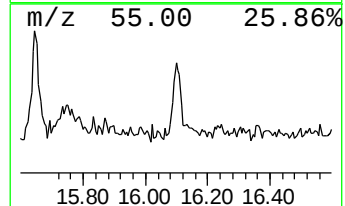
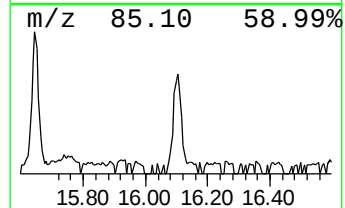
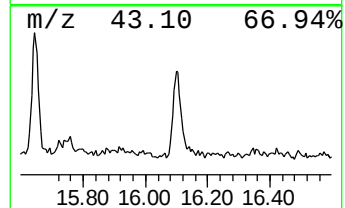
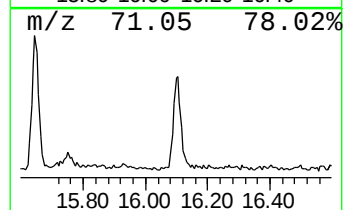
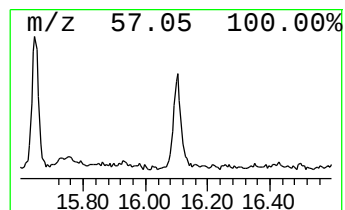
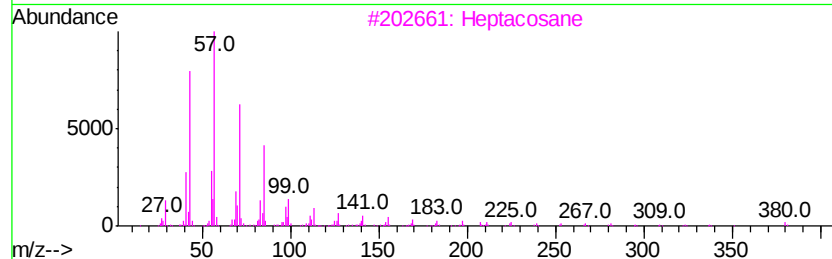
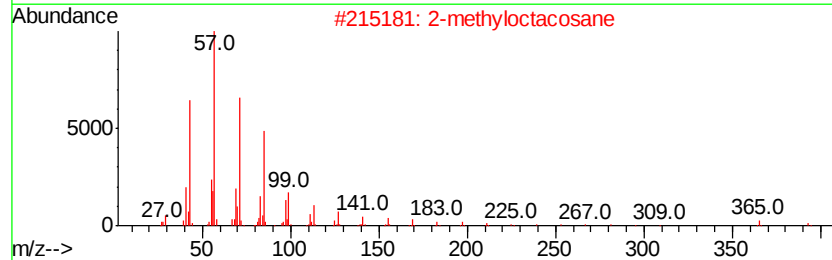
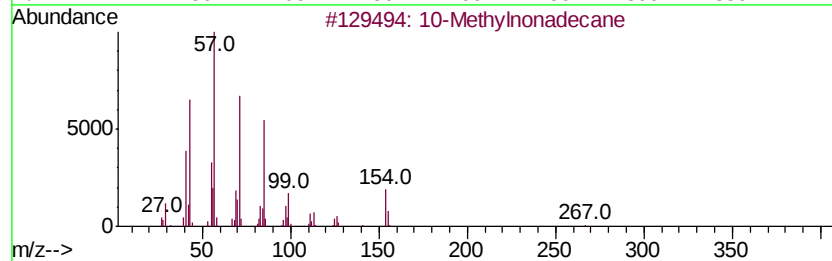
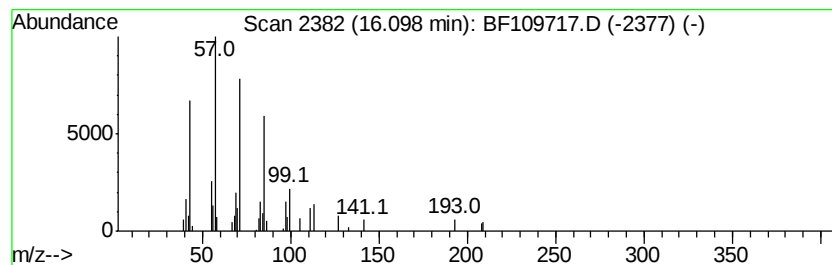
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 10-Methylnonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.55 ng	66856	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Methylnonadecane	282	C20H42	056862-62-5	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100918\
Data File : BF109717.D
Acq On : 10 Oct 2018 1:36
Operator : JU/SJ
Sample : J5329-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POND-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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...	4.90	2.8	ng	62757	1	6.70	456292	20.0
unknown6.47	6.47	83.6	ng	1906290	1	6.70	456292	20.0
1-Heptacosanol	13.69	5.8	ng	161596	5	13.83	560312	20.0
Heneicosane	14.90	2.1	ng	54269	6	15.22	523904	20.0
2-methyloctacosane	15.64	2.9	ng	75222	6	15.22	523904	20.0
10-Methylnonadecane	16.10	2.5	ng	66856	6	15.22	523904	20.0