

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
 Data File : BF102263.D
 Acq On : 20 Jan 2018 14:04
 Operator : SJ/JU
 Sample : J1115-11
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-35-2.5-3.0

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	4.934	479	484	492	rVB	186124	281907	7.01%	0.835%
2	5.339	547	553	556	rBV	3389525	3819852	94.97%	11.316%
3	6.363	718	727	739	rBV	3107761	4022213	100.00%	11.916%
4	6.492	744	749	752	rBV	3932488	3855564	95.86%	11.422%
5	6.722	784	788	791	rBV	1061821	955731	23.76%	2.831%
6	6.875	810	814	817	rBV	3180712	2960145	73.59%	8.770%
7	7.286	878	884	887	rBV	2314565	2443049	60.74%	7.238%
8	8.004	1001	1006	1009	rBV	1342070	1269545	31.56%	3.761%
9	9.080	1183	1189	1192	rBV	4075993	3677815	91.44%	10.896%
10	9.474	1251	1256	1259	rBV	609800	527925	13.13%	1.564%
11	9.686	1288	1292	1295	rBV	120665	90829	2.26%	0.269%
12	9.757	1299	1304	1307	rVB	1298129	1253356	31.16%	3.713%
13	10.186	1374	1377	1380	rVB	117282	93779	2.33%	0.278%
14	10.469	1420	1425	1427	rBV	40750	41245	1.03%	0.122%
15	10.545	1432	1438	1441	rBV	2110275	1955329	48.61%	5.793%
16	10.657	1454	1457	1465	rVB	94863	98286	2.44%	0.291%
17	11.104	1530	1533	1536	rBV2	62381	51084	1.27%	0.151%
18	11.239	1552	1556	1559	rBV	1133738	1054045	26.21%	3.123%
19	12.821	1821	1825	1829	rBV	2469864	2420532	60.18%	7.171%
20	13.715	1973	1977	1985	rBV	470912	473696	11.78%	1.403%
21	13.868	1999	2003	2007	rBV	855477	870736	21.65%	2.580%
22	14.351	2081	2085	2090	rBV3	50416	53046	1.32%	0.157%
23	15.292	2240	2245	2257	rBV2	675730	894436	22.24%	2.650%
24	15.733	2315	2320	2323	rBV	55121	84555	2.10%	0.250%
25	15.774	2323	2327	2334	rVB2	66111	105099	2.61%	0.311%
26	16.203	2395	2400	2404	rBV	61486	102914	2.56%	0.305%
27	16.756	2487	2494	2500	rBV2	58105	123524	3.07%	0.366%
28	17.409	2601	2605	2615	rVB4	48214	104715	2.60%	0.310%
29	18.186	2732	2737	2744	rVB5	28934	69919	1.74%	0.207%

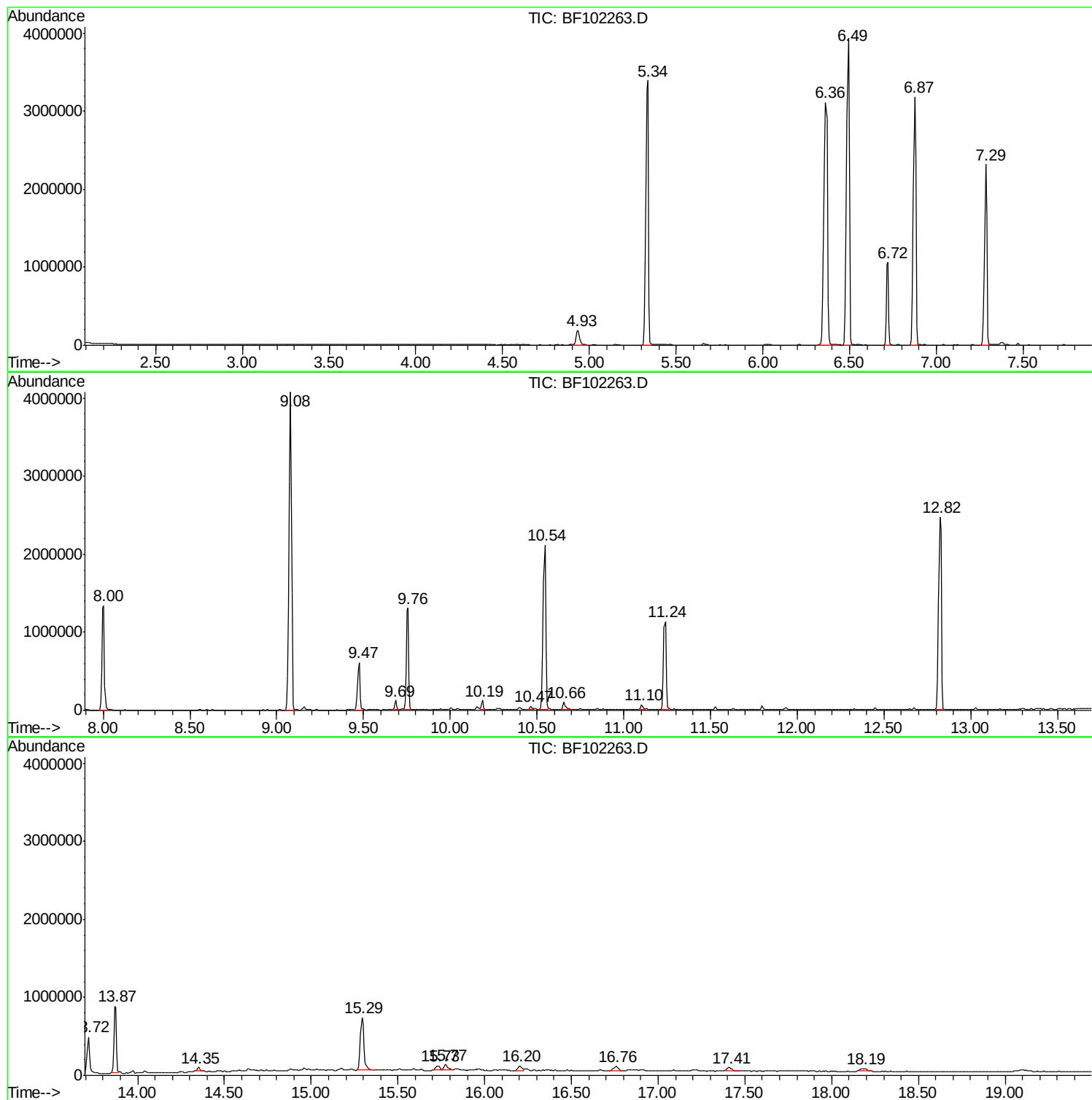
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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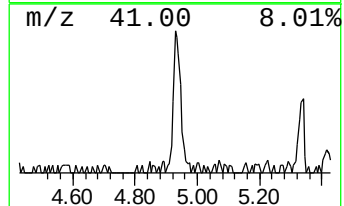
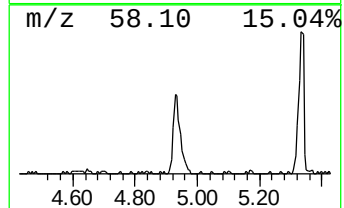
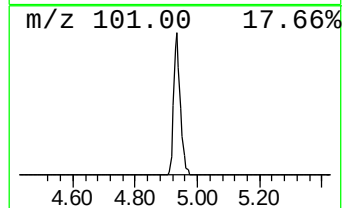
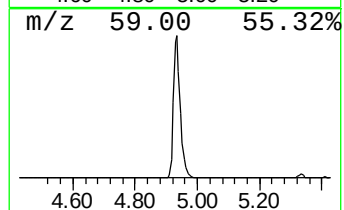
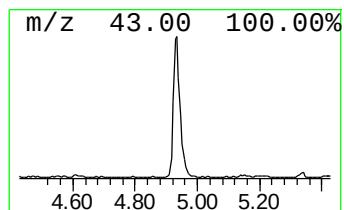
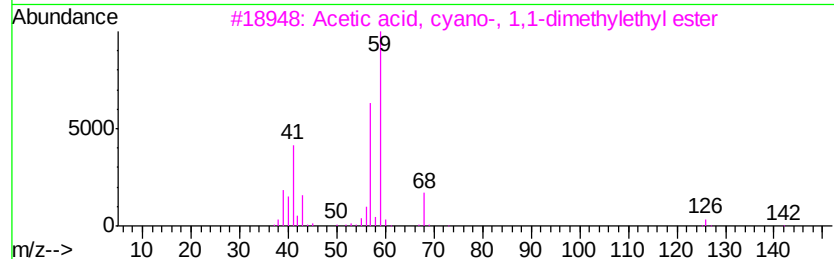
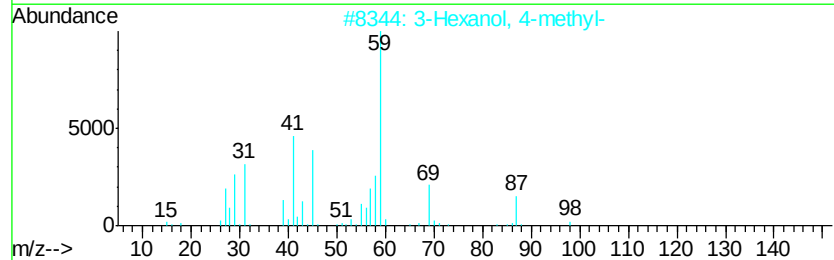
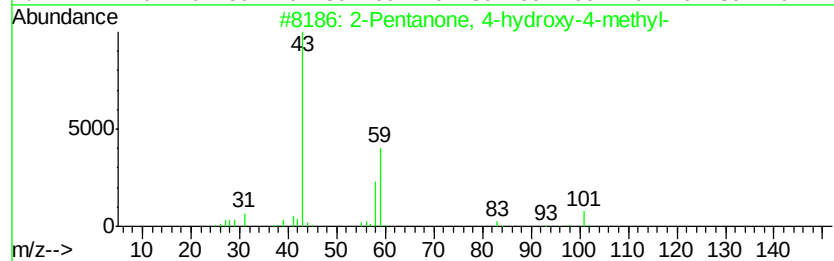
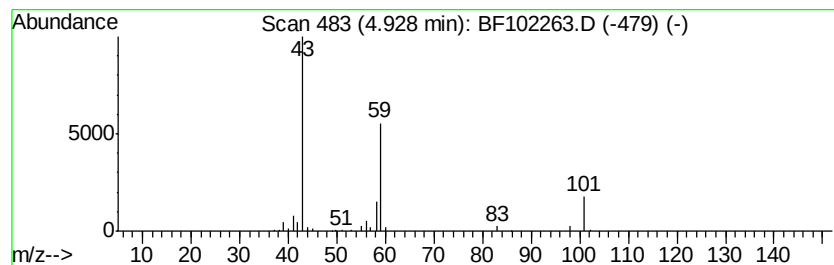
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	5.90 ng	281907	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	40
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			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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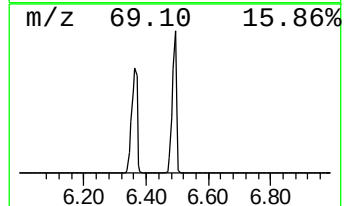
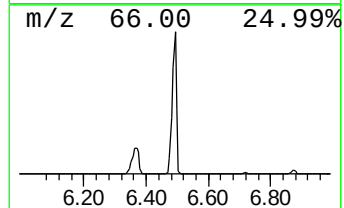
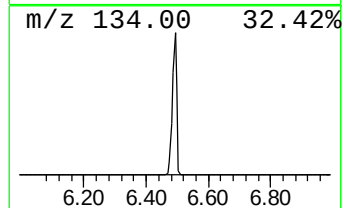
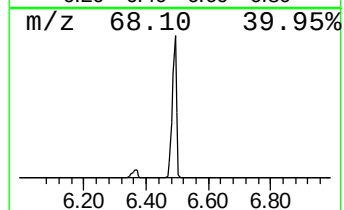
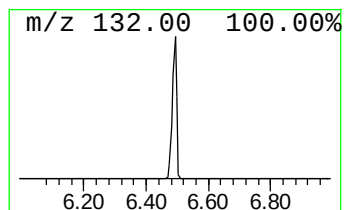
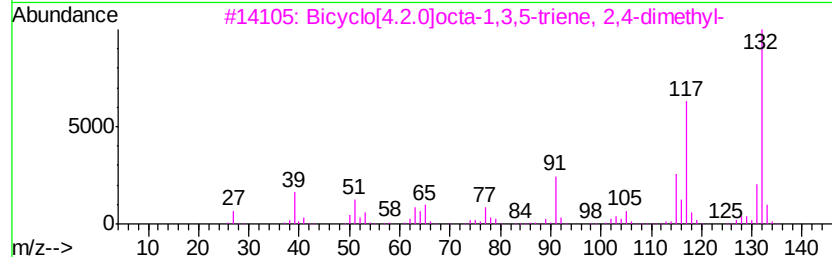
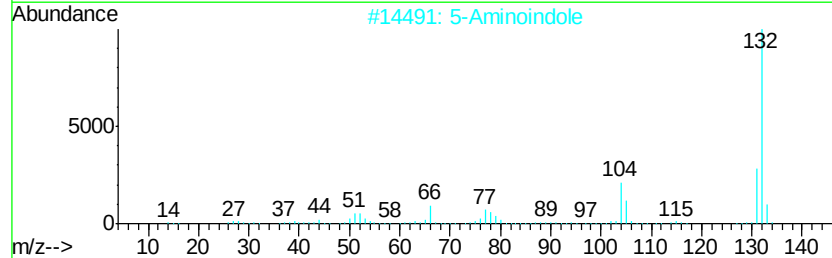
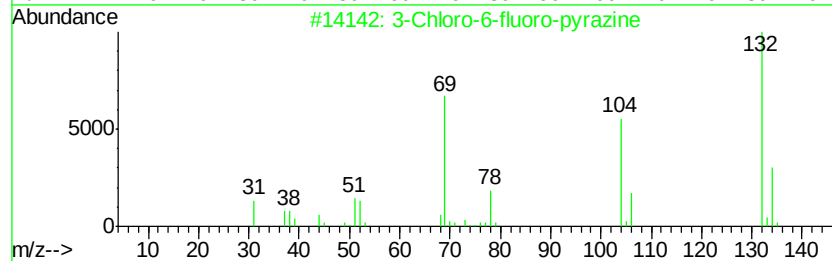
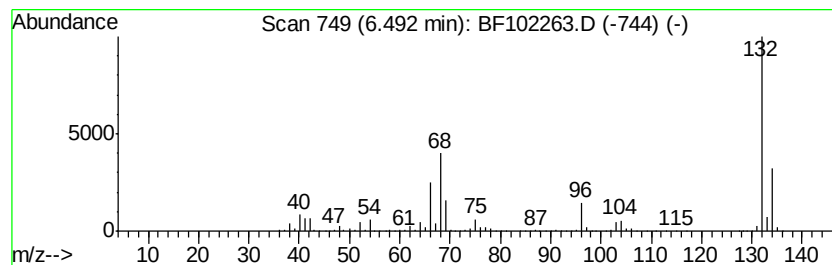
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	80.68 ng	3855560	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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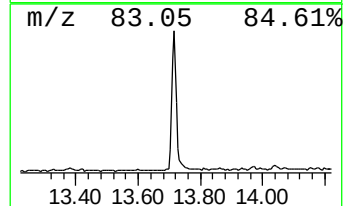
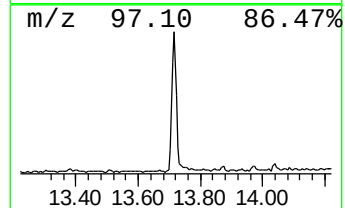
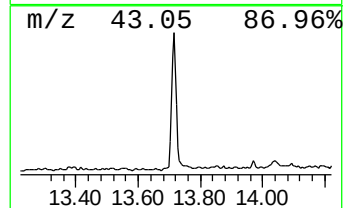
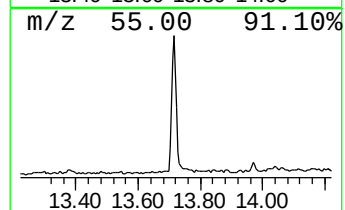
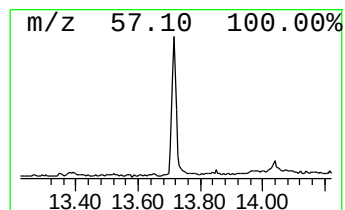
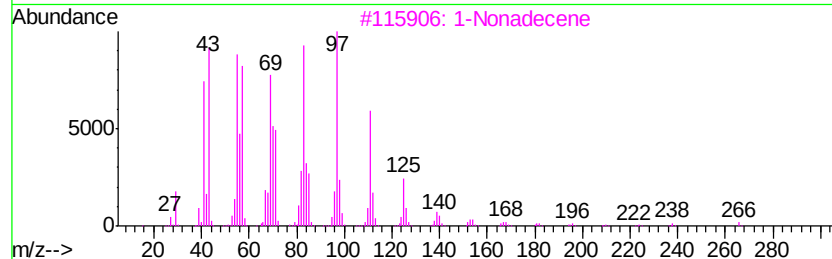
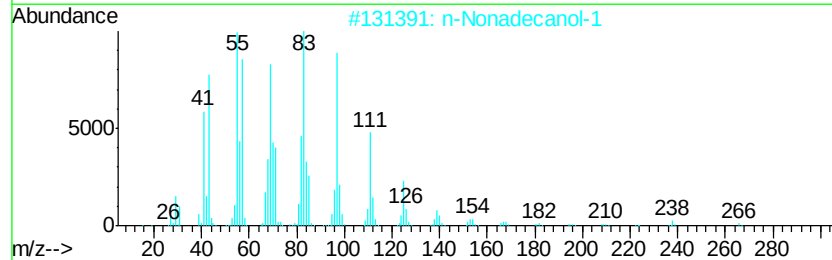
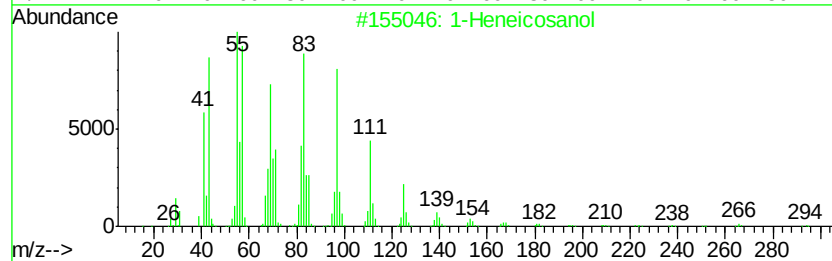
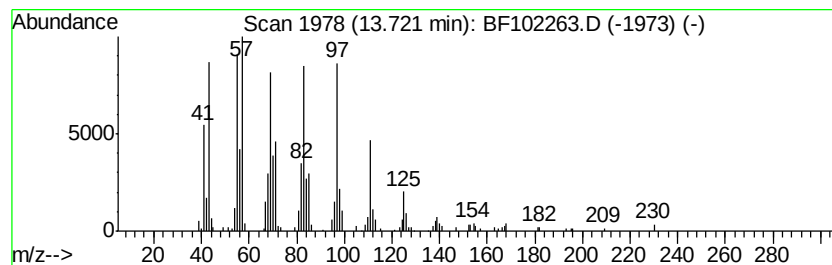
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.88 ng	473696	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		1-Nonadecene	266	C19H38	018435-45-5	94
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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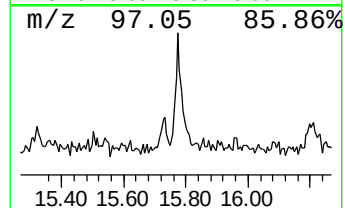
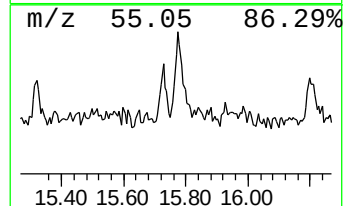
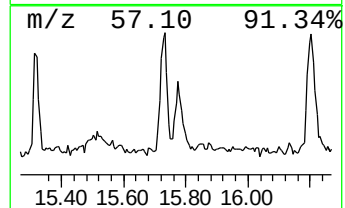
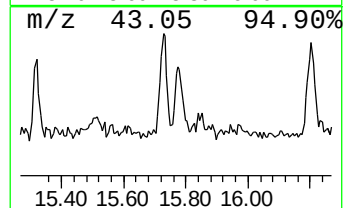
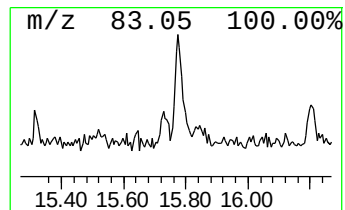
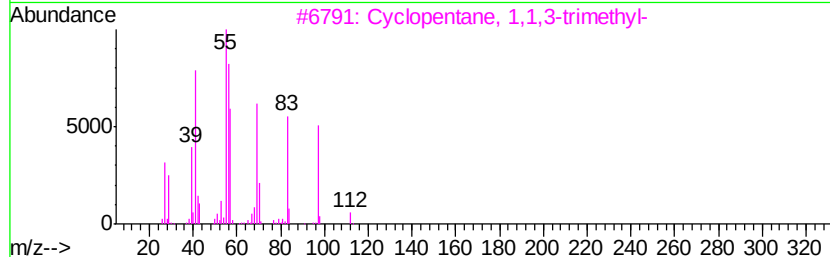
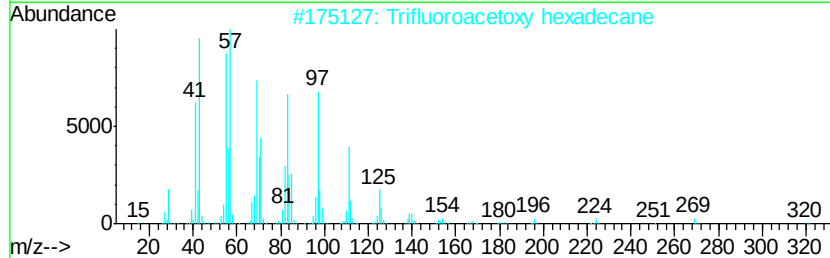
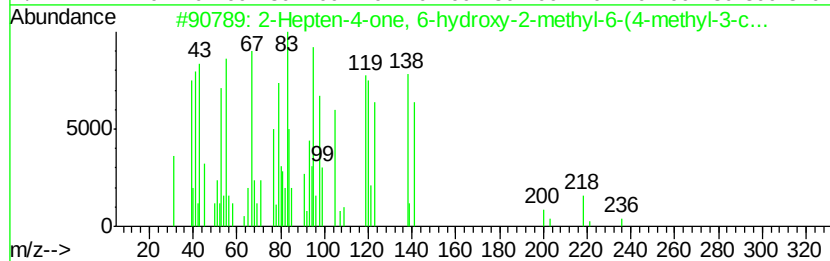
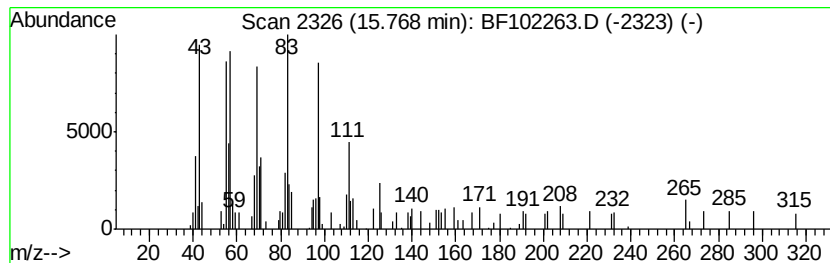
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Peak Number 5 2-Hepten-4-one, 6-hydroxy-2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.77	2.35 ng	105099	Perylene-d12	15.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	90	
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	70	
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	62	
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	60	
5	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56	



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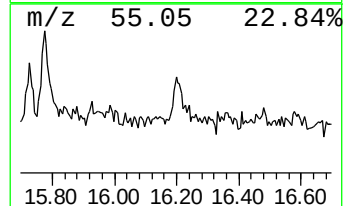
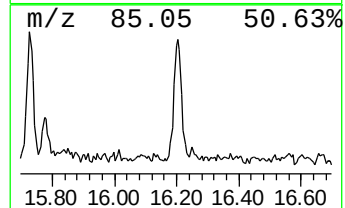
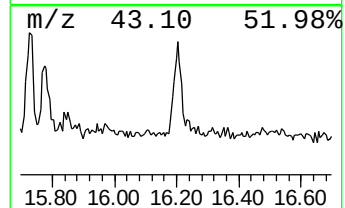
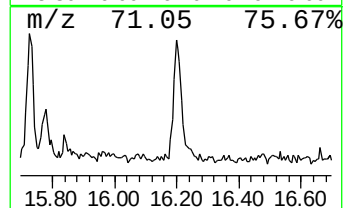
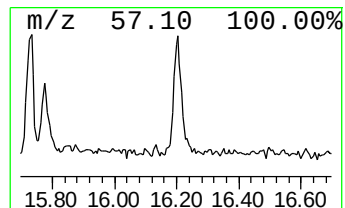
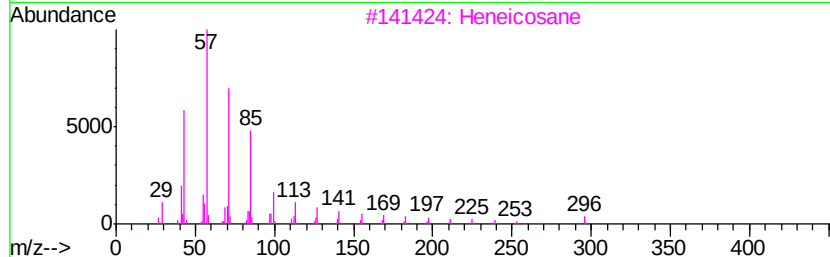
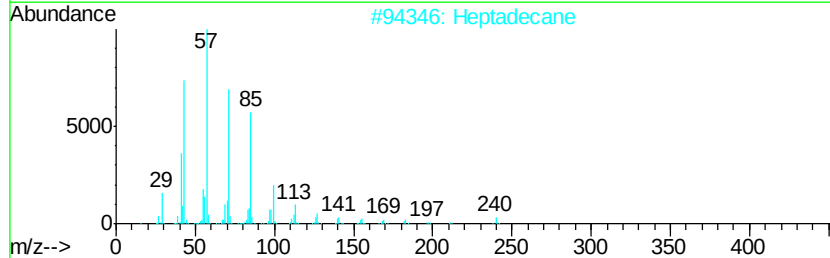
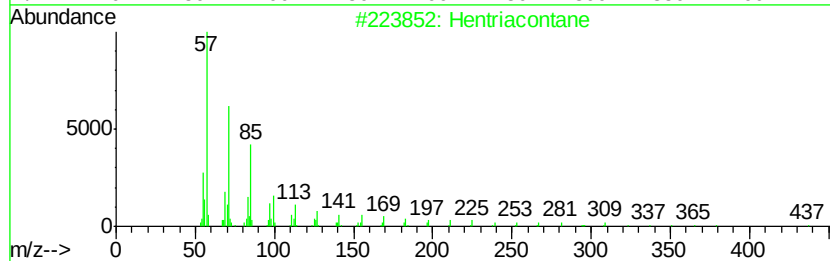
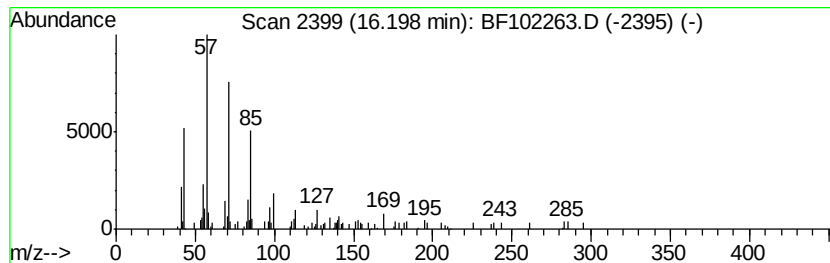
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	2.30 ng	102914	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	80
2	Heptadecane		240	C17H36	000629-78-7	80
3	Heneicosane		296	C21H44	000629-94-7	72
4	5-Ethyl-5-methylnonadecane		310	C22H46	1000360-42-7	72
5	Octadecane		254	C18H38	000593-45-3	64



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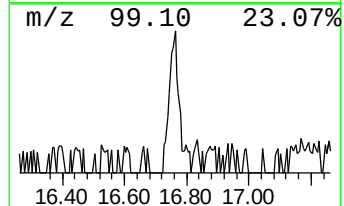
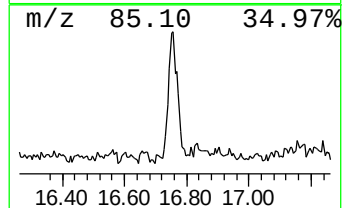
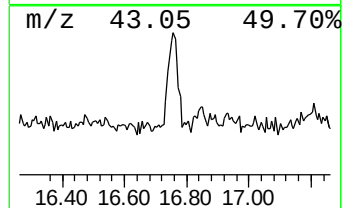
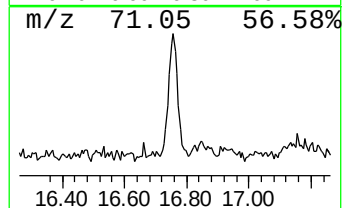
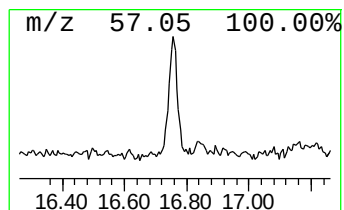
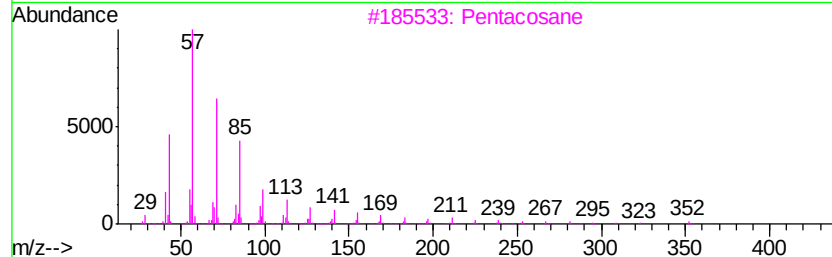
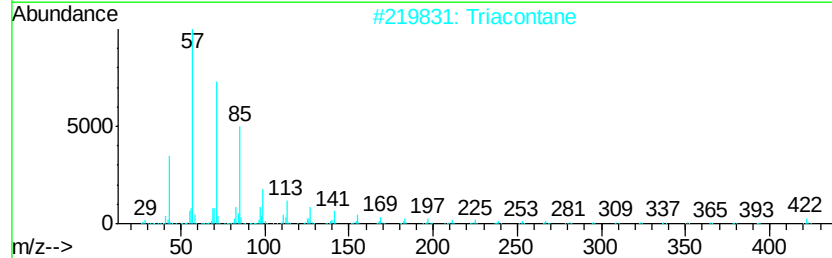
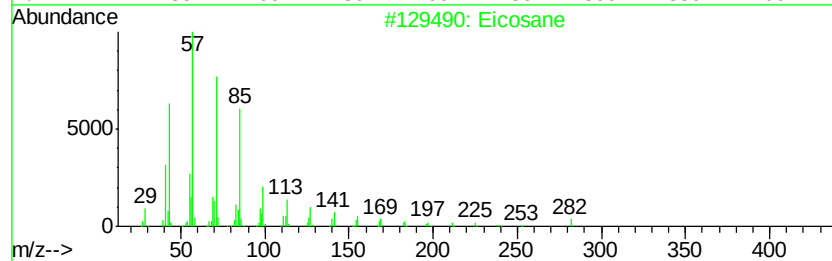
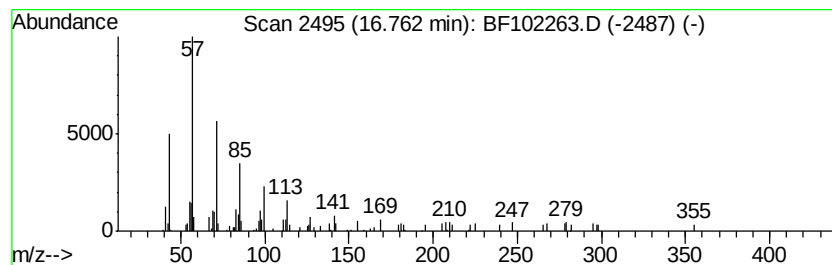
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	2.76 ng	123524	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	98
2	Triacontane		422	C30H62	000638-68-6	87
3	Pentacosane		352	C25H52	000629-99-2	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Heptacosane		380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102263.D
Acq On : 20 Jan 2018 14:04
Operator : SJ/JU
Sample : J1115-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-35-2.5-3.0

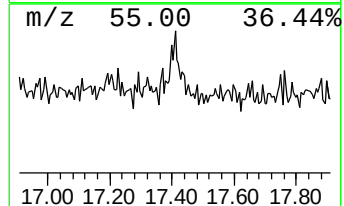
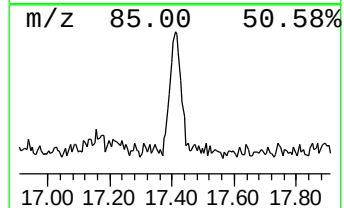
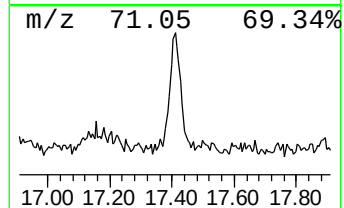
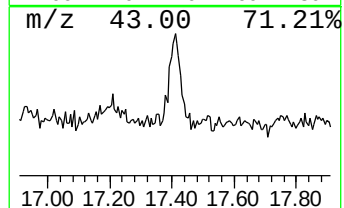
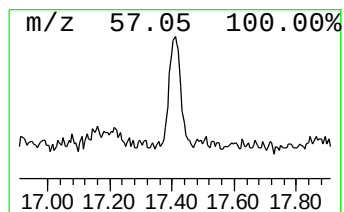
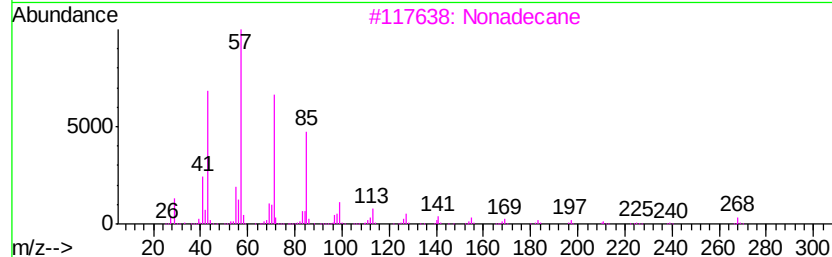
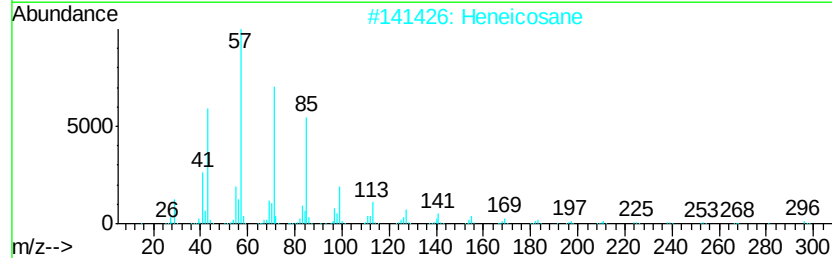
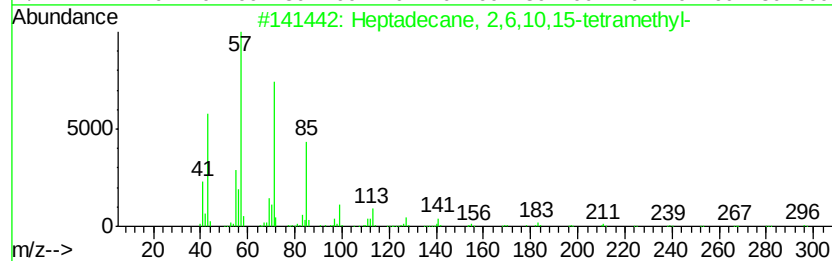
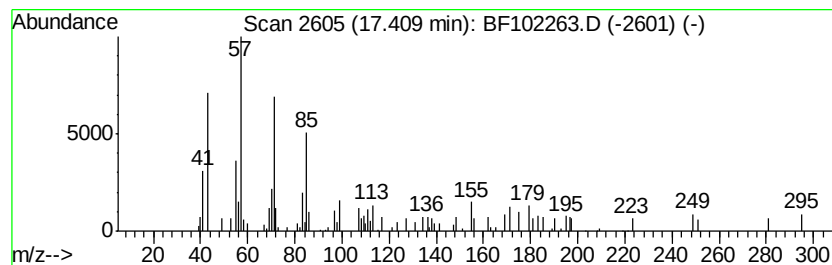
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.41 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	2.34 ng	104715	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	46
2		Heneicosane	296	C21H44	000629-94-7	46
3		Nonadecane	268	C19H40	000629-92-5	46
4		2-methyltetracosane	352	C25H52	1000376-72-6	46
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102263.D
Acq On : 20 Jan 2018 14:04
Operator : SJ/JU
Sample : J1115-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-35-2.5-3.0

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	281907	1	6.72	955731	20.0
unknown6.49	6.49	80.7	ng	3855560	1	6.72	955731	20.0
1-Heneicosanol	13.72	10.9	ng	473696	5	13.87	870736	20.0
2-Hepten-4-one, 6...	15.77	2.4	ng	105099	6	15.29	894436	20.0
Hentriacontane	16.20	2.3	ng	102914	6	15.29	894436	20.0
Eicosane	16.76	2.8	ng	123524	6	15.29	894436	20.0
unknown17.41	17.41	2.3	ng	104715	6	15.29	894436	20.0