

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082817\
 Data File : BF098100.D
 Acq On : 29 Aug 2017 7:30
 Operator : SJ/JU
 Sample : I4961-06
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-12-COMP

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-BF081517.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	480	484	499	rVB	186159	247378	9.23%	1.017%
2	5.351	550	555	558	rBV	2502722	2495640	93.13%	10.258%
3	6.381	724	730	747	rVB	2419596	2679779	100.00%	11.015%
4	6.510	747	752	755	rBV	2736605	2483446	92.67%	10.208%
5	6.740	787	791	795	rBV	800514	638849	23.84%	2.626%
6	6.898	813	818	821	rBV	1936304	1863776	69.55%	7.661%
7	7.304	882	887	890	rBV	1740907	1578078	58.89%	6.486%
8	8.022	1005	1009	1022	rBV	936378	825913	30.82%	3.395%
9	9.098	1187	1192	1195	rBV	2782041	2446735	91.30%	10.057%
10	9.492	1255	1259	1268	rVB	306332	260938	9.74%	1.073%
11	9.775	1302	1307	1311	rBV	936925	830609	31.00%	3.414%
12	10.210	1378	1381	1384	rVB	37130	29696	1.11%	0.122%
13	10.563	1436	1441	1453	rBV	1463262	1441084	53.78%	5.923%
14	10.680	1458	1461	1468	rVB	46395	43470	1.62%	0.179%
15	11.257	1555	1559	1561	rBV	955204	824954	30.78%	3.391%
16	11.280	1561	1563	1566	rVB	85174	68707	2.56%	0.282%
17	11.557	1606	1610	1613	rVB	34579	31939	1.19%	0.131%
18	12.463	1760	1764	1767	rBV	94986	79918	2.98%	0.328%
19	12.692	1800	1803	1806	rVB	80702	71898	2.68%	0.296%
20	12.839	1824	1828	1832	rBV	2083730	2063760	77.01%	8.483%
21	13.739	1977	1981	1988	rBV2	161271	187913	7.01%	0.772%
22	13.886	2001	2006	2009	rBV	837800	825553	30.81%	3.393%
23	13.910	2009	2010	2016	rVB	50802	40591	1.51%	0.167%
24	14.368	2085	2088	2095	rVB2	95628	116870	4.36%	0.480%
25	14.904	2175	2179	2181	rBV	36033	52785	1.97%	0.217%
26	14.986	2189	2193	2194	rBV	54007	62325	2.33%	0.256%
27	15.010	2194	2197	2203	rVB	104480	138042	5.15%	0.567%
28	15.245	2235	2237	2241	rVB2	30801	35072	1.31%	0.144%
29	15.310	2243	2248	2251	rVV	611030	745538	27.82%	3.064%
30	15.345	2251	2254	2257	rVV2	99526	126159	4.71%	0.519%
31	15.380	2258	2260	2267	rVB7	23565	30715	1.15%	0.126%
32	15.757	2319	2324	2328	rBV	113243	170208	6.35%	0.700%
33	15.804	2328	2332	2341	rVV4	37717	72171	2.69%	0.297%
34	16.227	2399	2404	2410	rVB	126848	194411	7.25%	0.799%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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35	16.780	2492	2498	2505	rBV2	94402	188390	7.03%	0.774%
36	17.439	2604	2610	2620	rVB3	80442	194878	7.27%	0.801%
37	18.209	2735	2741	2752	rVB4	49325	140480	5.24%	0.577%

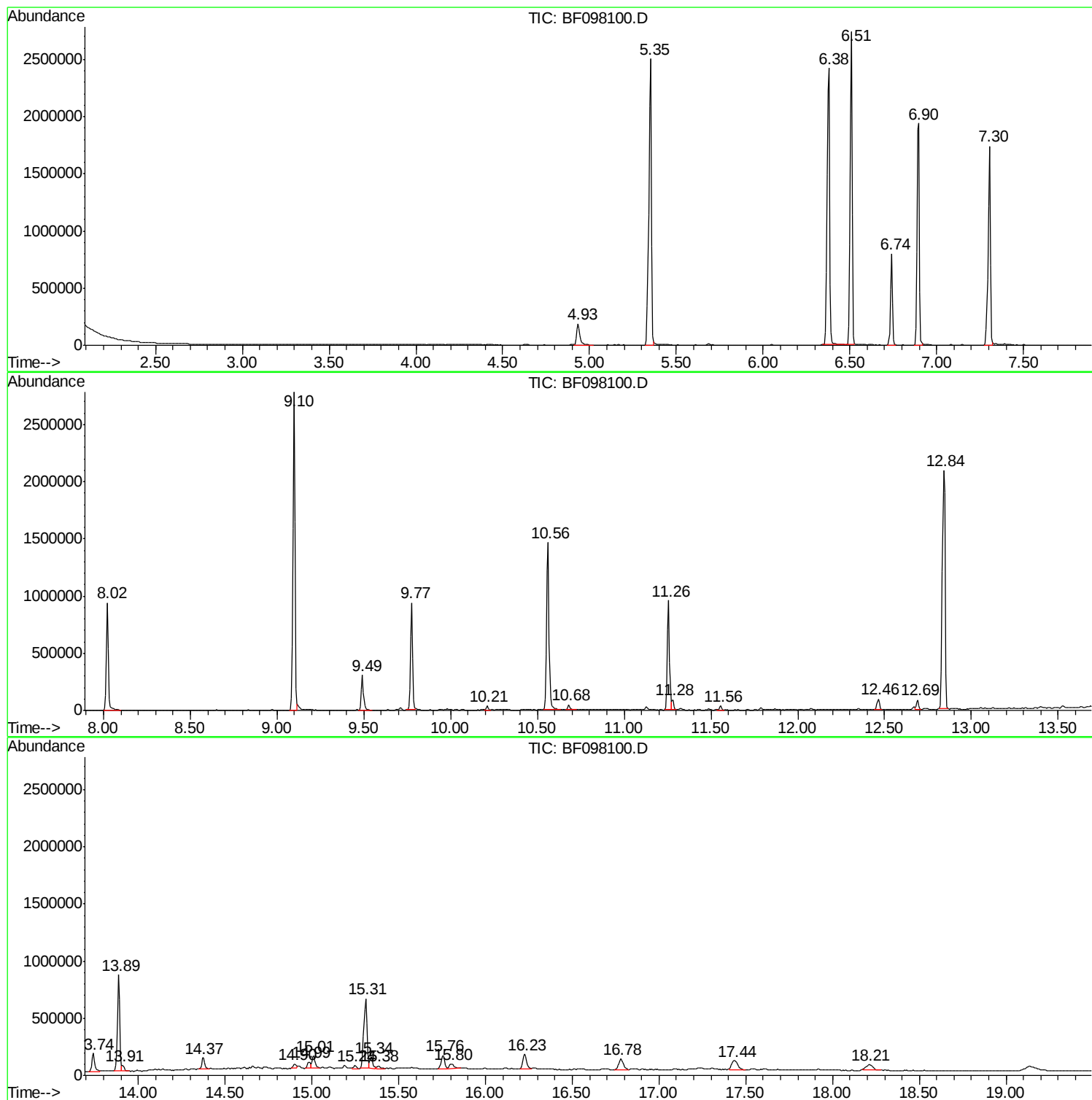
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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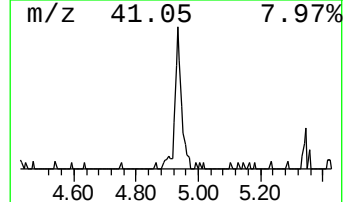
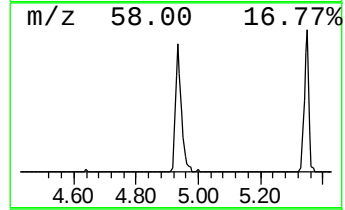
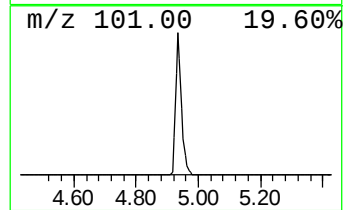
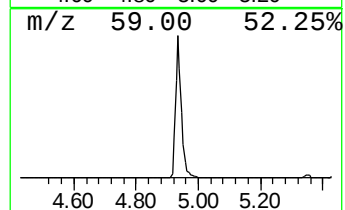
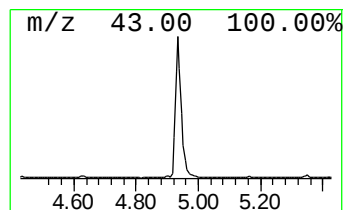
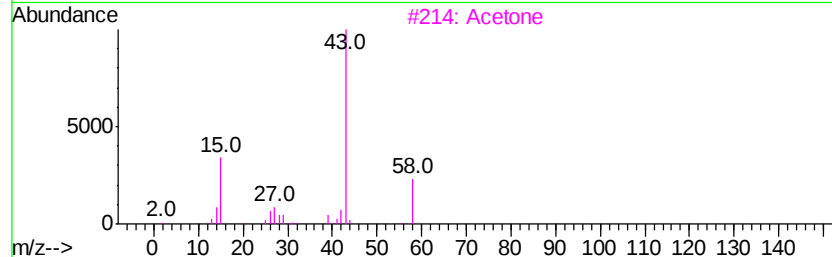
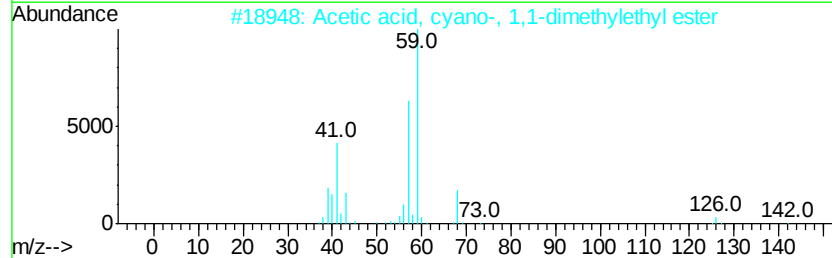
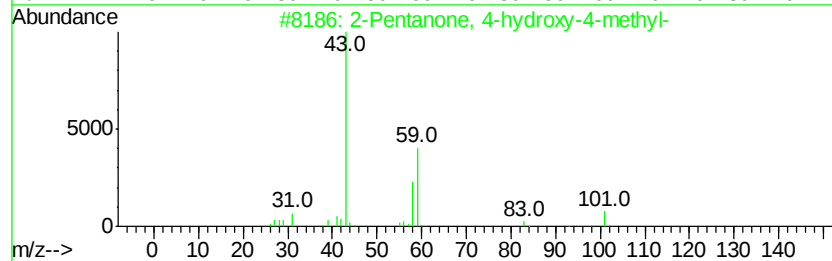
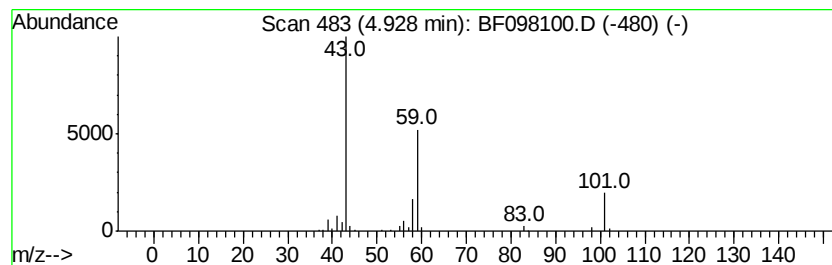
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.74 ng	247378	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3			Acetone	58	C3H6O	000067-64-1	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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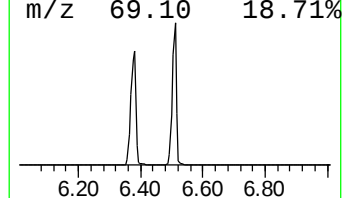
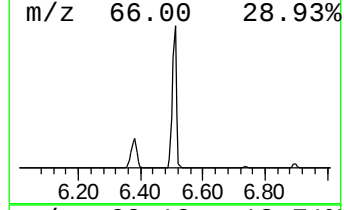
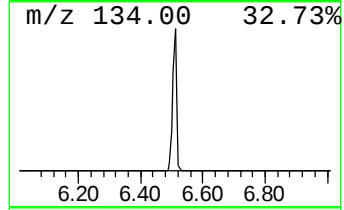
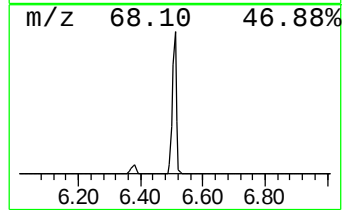
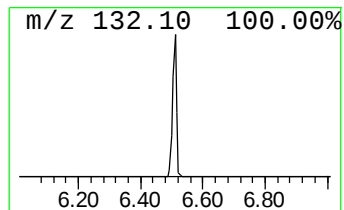
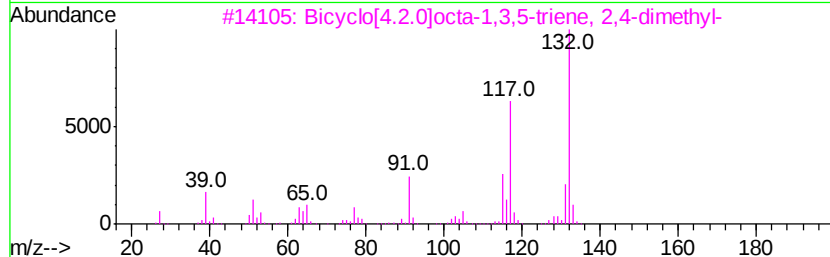
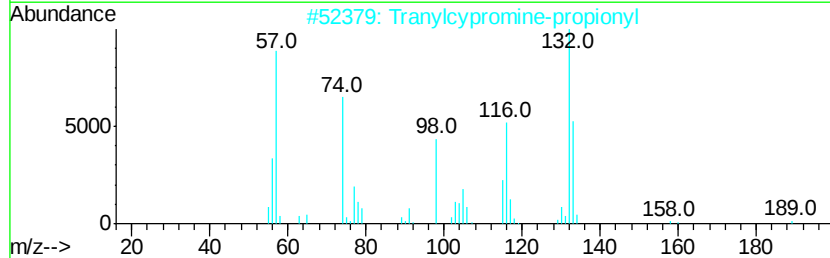
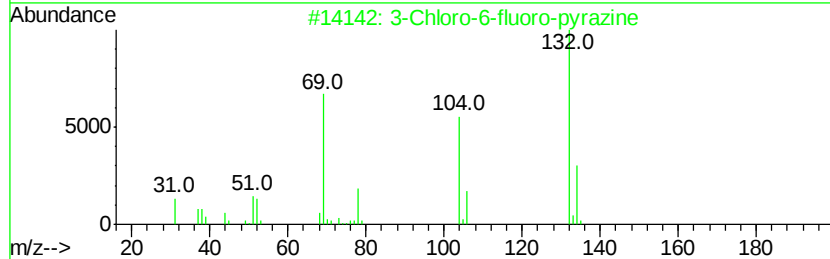
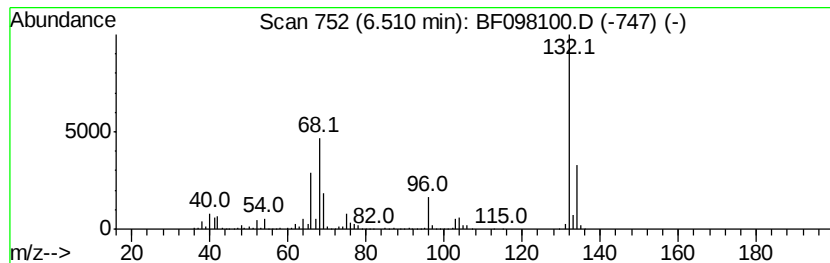
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	77.75 ng	2483450	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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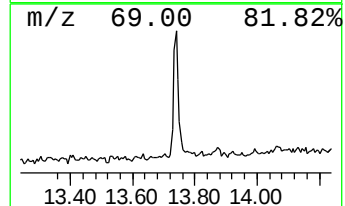
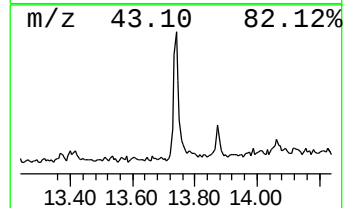
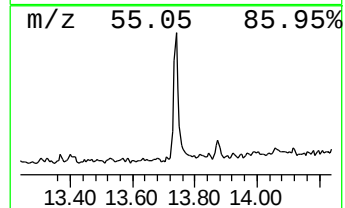
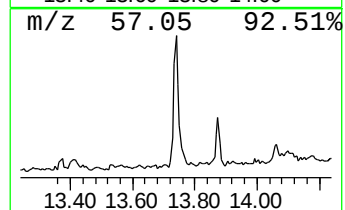
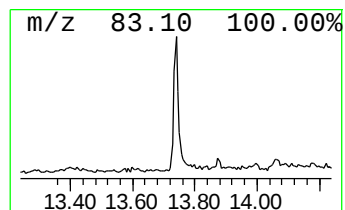
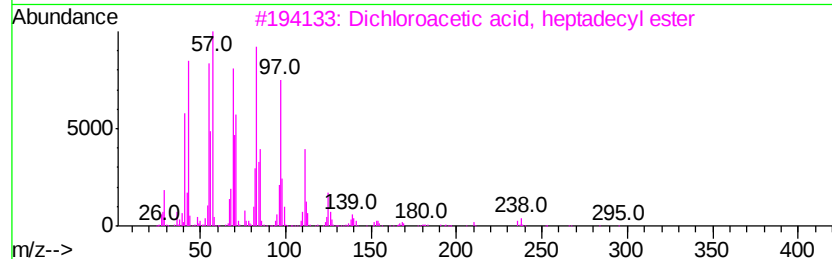
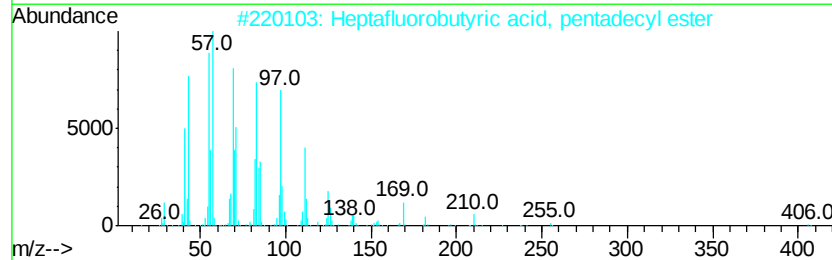
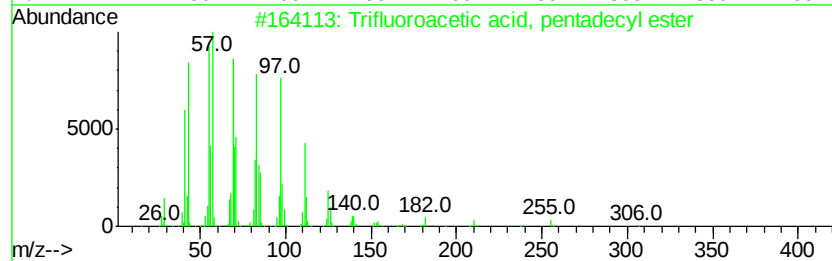
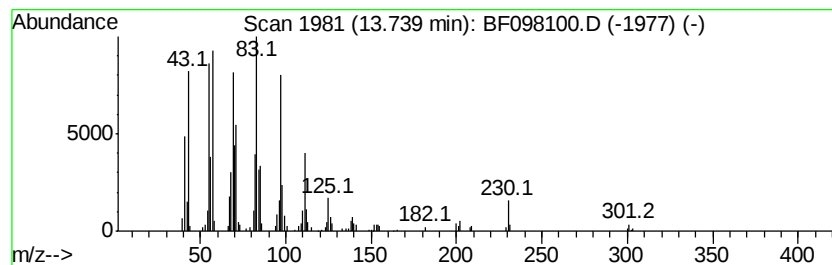
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.55 ng	187913	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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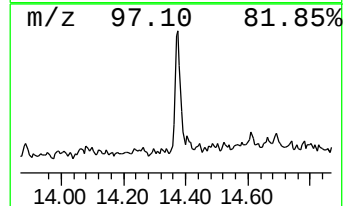
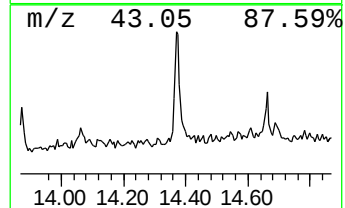
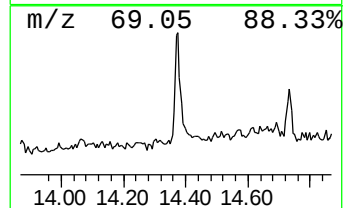
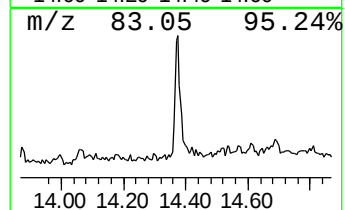
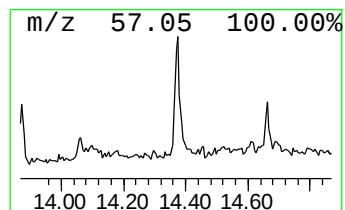
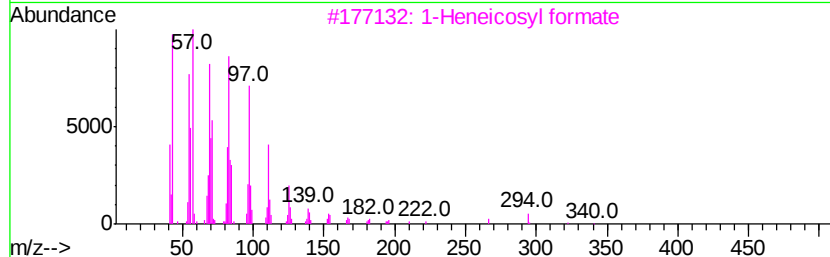
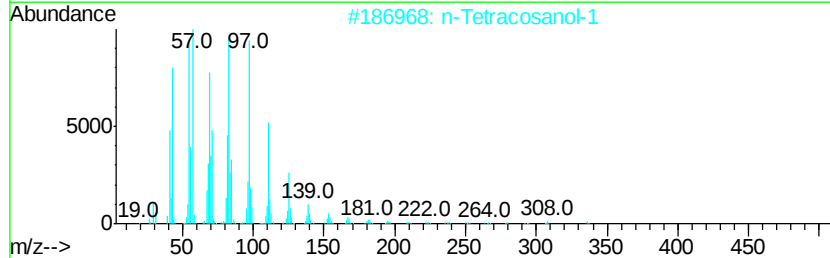
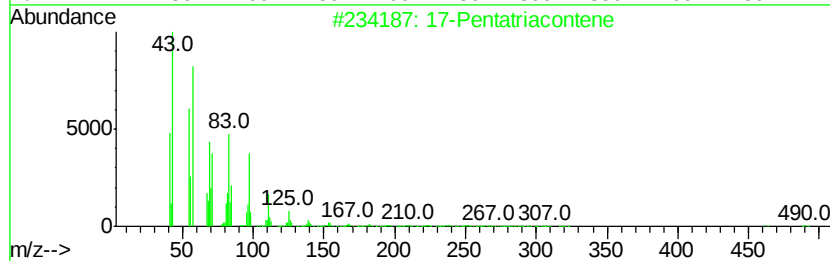
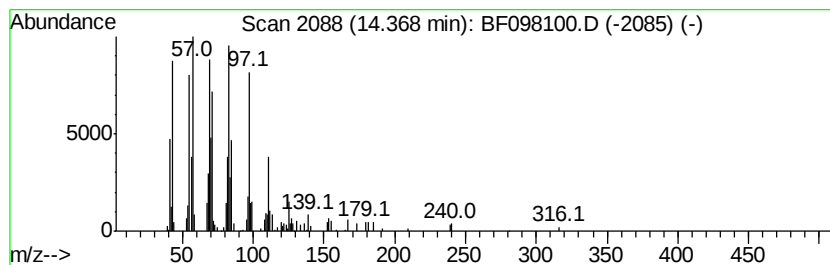
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 17-Pentatriacontene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.83 ng	116870	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4		Behenic alcohol	326	C22H46O	000661-19-8	83
5		1-Heptacosanol	396	C27H56O	002004-39-9	70



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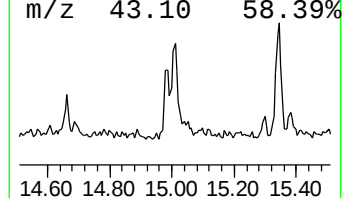
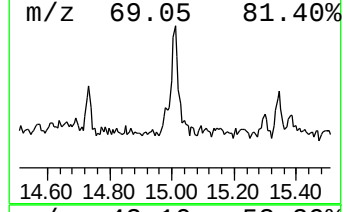
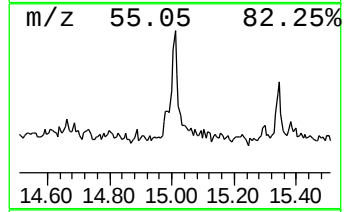
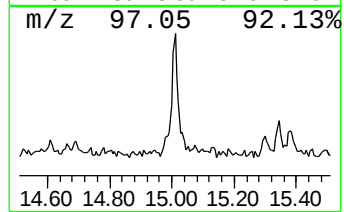
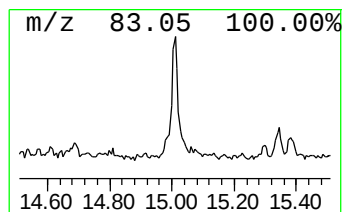
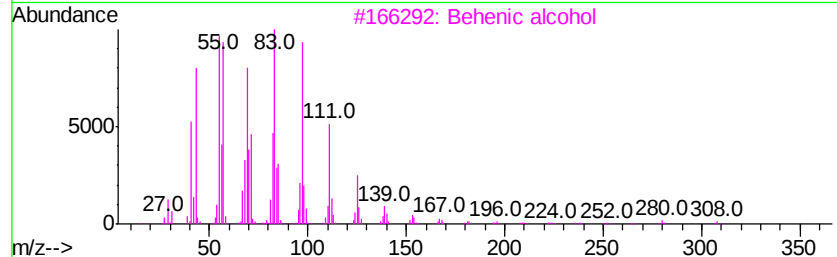
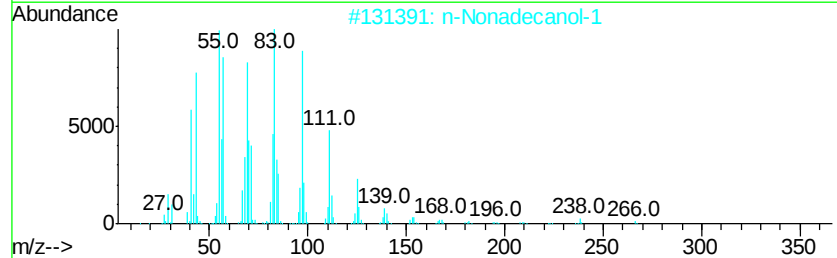
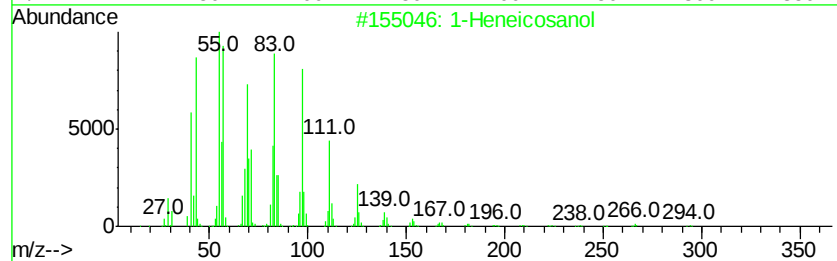
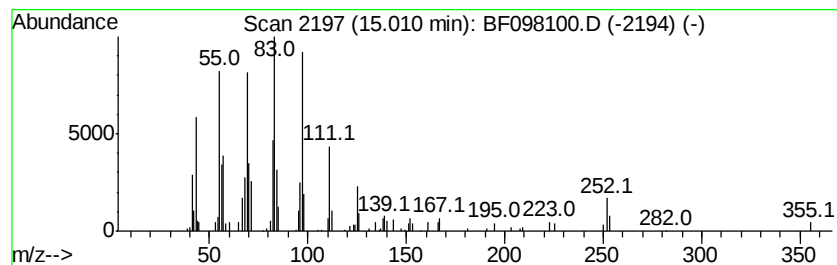
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Peak Number 6 1-Heneicosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.01	3.70 ng	138042	Perylene-d12	15.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	Cyclopentadecane	210	C15H30	000295-48-7	83
5	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082817\
Data File : BF098100.D
Acq On : 29 Aug 2017 7:30
Operator : SJ/JU
Sample : I4961-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

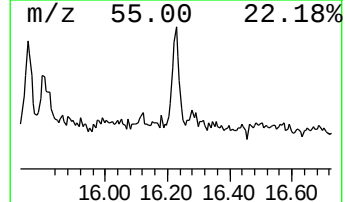
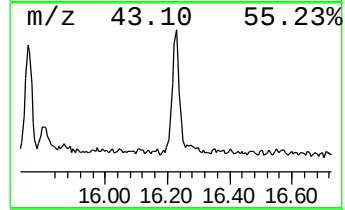
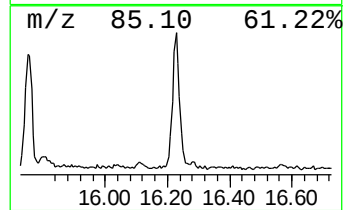
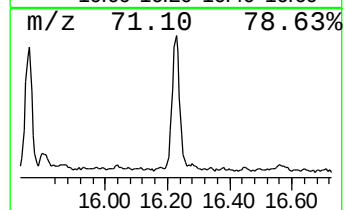
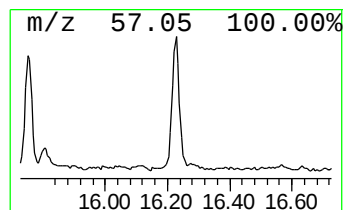
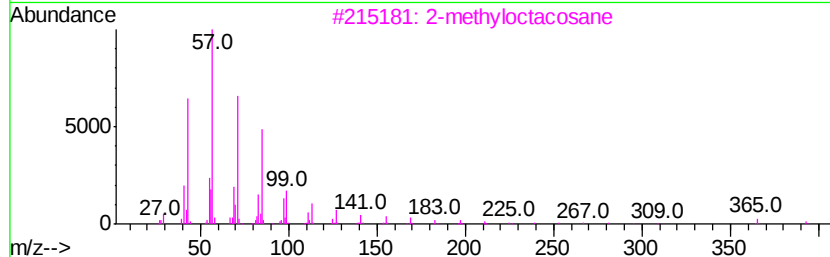
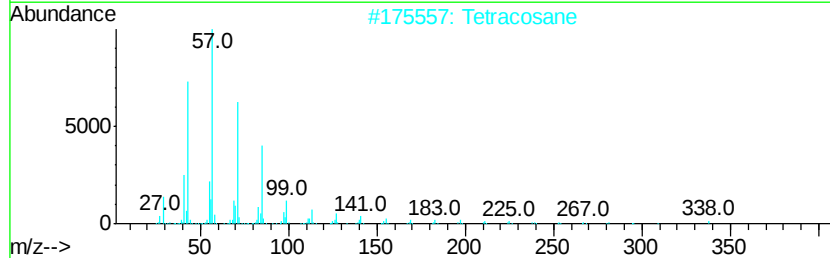
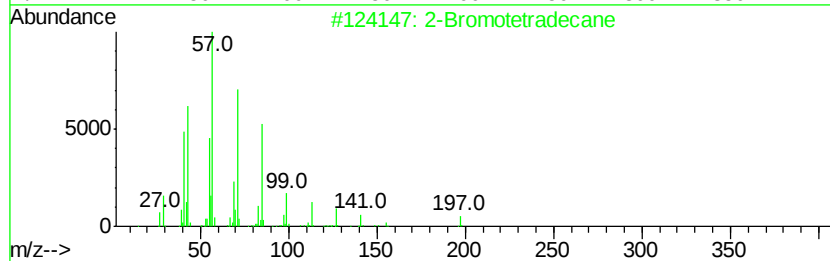
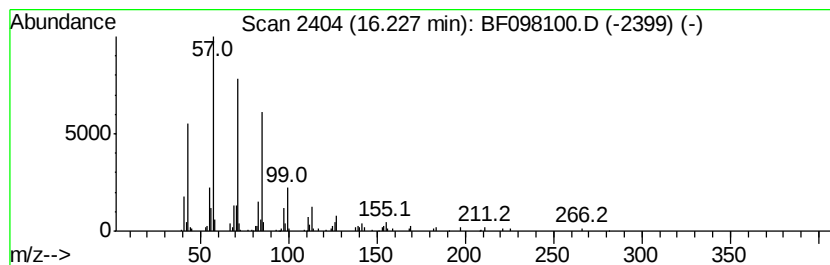
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Bromotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	5.22 ng	194411	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
2		Tetracosane	338	C24H50	000646-31-1	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	86
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5		Dodecane, 3-methyl-	184	C13H28	017312-57-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082817\
Data File : BF098100.D
Acq On : 29 Aug 2017 7:30
Operator : SJ/JU
Sample : I4961-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

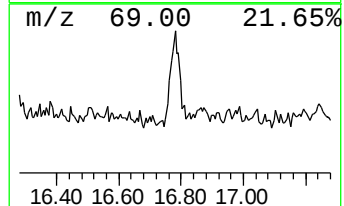
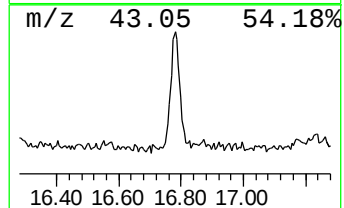
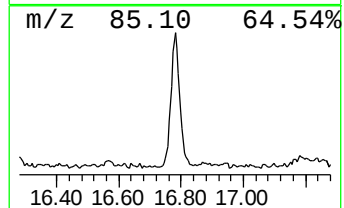
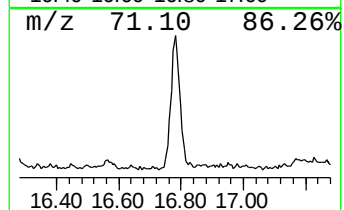
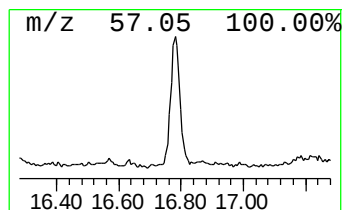
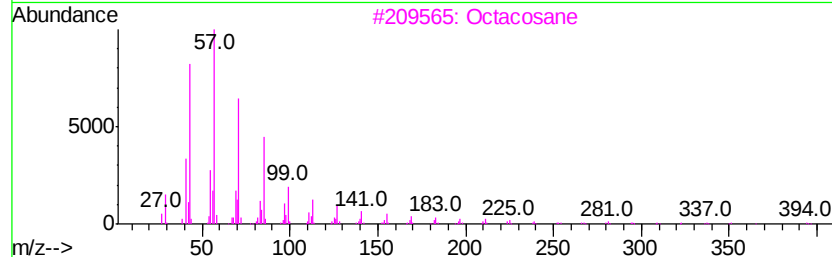
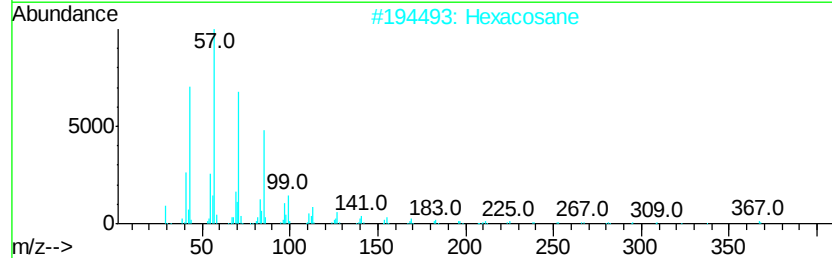
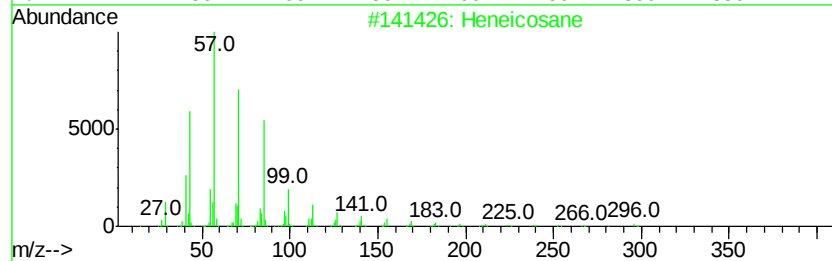
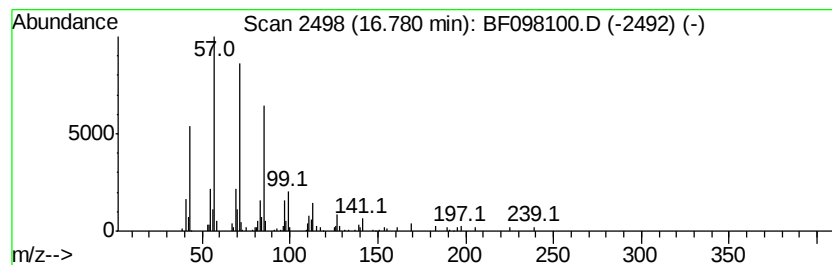
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	5.05 ng	188390	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Octacosane		394	C28H58	000630-02-4	91
4	triacontane		422	C30H62	000638-68-6	91
5	Hentriacontane		437	C31H64	000630-04-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082817\
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Acq On : 29 Aug 2017 7:30
Operator : SJ/JU
Sample : I4961-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

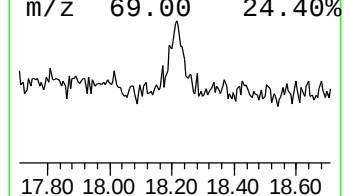
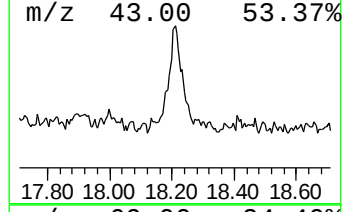
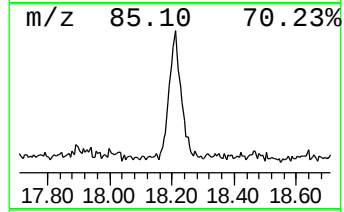
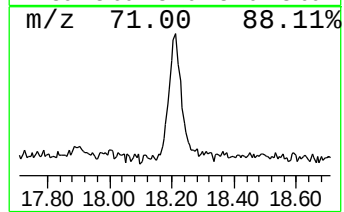
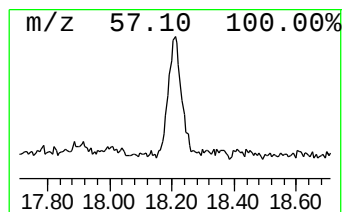
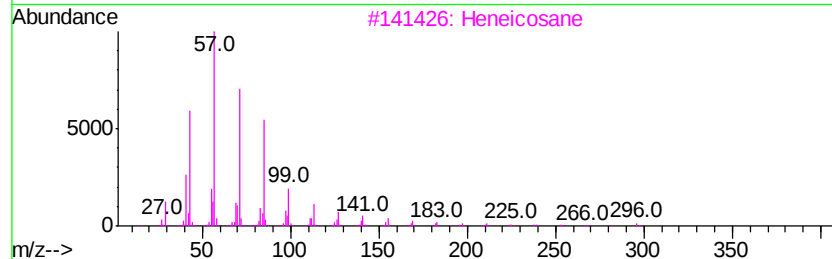
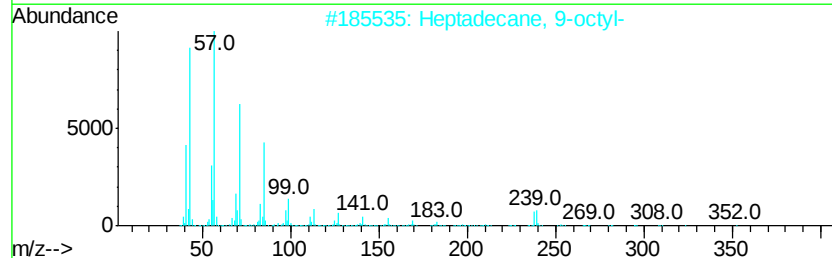
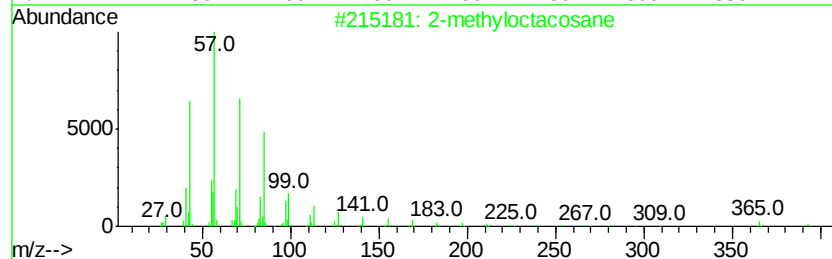
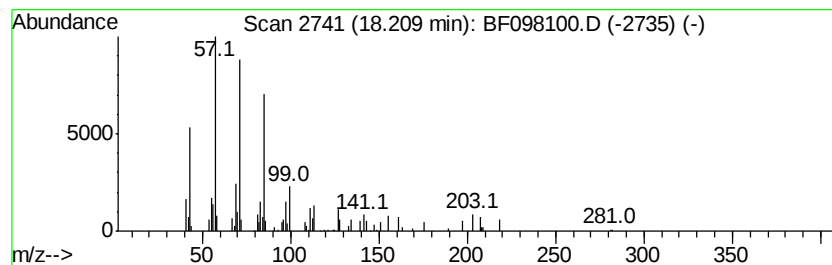
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	3.77 ng	140480	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	83
5		Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082817\
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Acq On : 29 Aug 2017 7:30
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Sample : I4961-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	7.7	ng	247378	1	6.74	638849	20.0
unknown6.51	6.51	77.8	ng	2483450	1	6.74	638849	20.0
Trifluoroacetic a...	13.74	4.5	ng	187913	5	13.89	825553	20.0
17-Pentatriacontene	14.37	2.8	ng	116870	5	13.89	825553	20.0
1-Heneicosanol	15.01	3.7	ng	138042	6	15.31	745538	20.0
2-Bromotetradecane	16.23	5.2	ng	194411	6	15.31	745538	20.0
Heneicosane	16.78	5.0	ng	188390	6	15.31	745538	20.0
2-methyloctacosane	18.21	3.8	ng	140480	6	15.31	745538	20.0