

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
 Data File : BF099925.D
 Acq On : 28 Oct 2017 18:54
 Operator : SJ/JU
 Sample : I6141-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-B-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-BF102317.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	5.004	493	496	519	rBV	147413	236424	14.53%	1.505%
2	5.410	562	565	589	rBV	1379144	1535541	94.40%	9.776%
3	6.434	735	739	751	rBV	1388422	1511681	92.93%	9.624%
4	6.557	757	760	775	rVB	1776338	1626630	100.00%	10.356%
5	6.787	796	799	808	rBV	545090	485790	29.86%	3.093%
6	6.939	821	825	843	rBV	1385195	1224654	75.29%	7.797%
7	7.357	892	896	914	rBV	1013036	955182	58.72%	6.081%
8	8.069	1013	1017	1032	rBV	766177	674093	41.44%	4.292%
9	9.139	1195	1199	1202	rBV	1986217	1624480	99.87%	10.342%
10	9.539	1264	1267	1278	rVB	239550	195895	12.04%	1.247%
11	9.822	1311	1315	1320	rBV	846878	702397	43.18%	4.472%
12	10.616	1446	1450	1459	rBV	825723	755010	46.42%	4.807%
13	10.710	1463	1466	1473	rVB	34939	33372	2.05%	0.212%
14	11.310	1565	1568	1572	rBV	612336	591423	36.36%	3.765%
15	11.339	1572	1573	1577	rVB	41528	25855	1.59%	0.165%
16	11.827	1651	1656	1659	rBV2	20061	23062	1.42%	0.147%
17	12.533	1772	1776	1780	rBV	50269	43649	2.68%	0.278%
18	12.763	1813	1815	1820	rVB	40646	36294	2.23%	0.231%
19	12.892	1833	1837	1840	rBV	1227842	1023065	62.89%	6.513%
20	13.774	1983	1987	1993	rBV	54150	61364	3.77%	0.391%
21	13.963	2015	2019	2022	rBV	462726	439015	26.99%	2.795%
22	14.404	2090	2094	2101	rBV5	18960	36392	2.24%	0.232%
23	14.698	2141	2144	2149	rBV2	20465	23096	1.42%	0.147%
24	15.021	2193	2199	2204	rBV3	60358	87063	5.35%	0.554%
25	15.157	2219	2222	2226	rBV2	26343	32392	1.99%	0.206%
26	15.251	2234	2238	2243	rVB	38988	48373	2.97%	0.308%
27	15.386	2255	2261	2264	rBV2	81825	115010	7.07%	0.732%
28	15.421	2264	2267	2280	rVB	383583	471965	29.01%	3.005%
29	15.804	2328	2332	2338	rVB	102167	148923	9.16%	0.948%
30	16.286	2408	2414	2422	rBV	116251	208604	12.82%	1.328%
31	16.739	2487	2491	2499	rVB2	23492	46290	2.85%	0.295%
32	16.856	2504	2511	2518	rBV	90990	185399	11.40%	1.180%
33	17.433	2604	2609	2615	rVV8	12625	25275	1.55%	0.161%
34	17.527	2618	2625	2635	rVB2	82070	194586	11.96%	1.239%

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SP-1-B-COMP

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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35	18.315	2752	2759	2774	rVB3	50022	150777	9.27%	0.960%
36	19.262	2911	2920	2932	rBV5	37414	128469	7.90%	0.818%

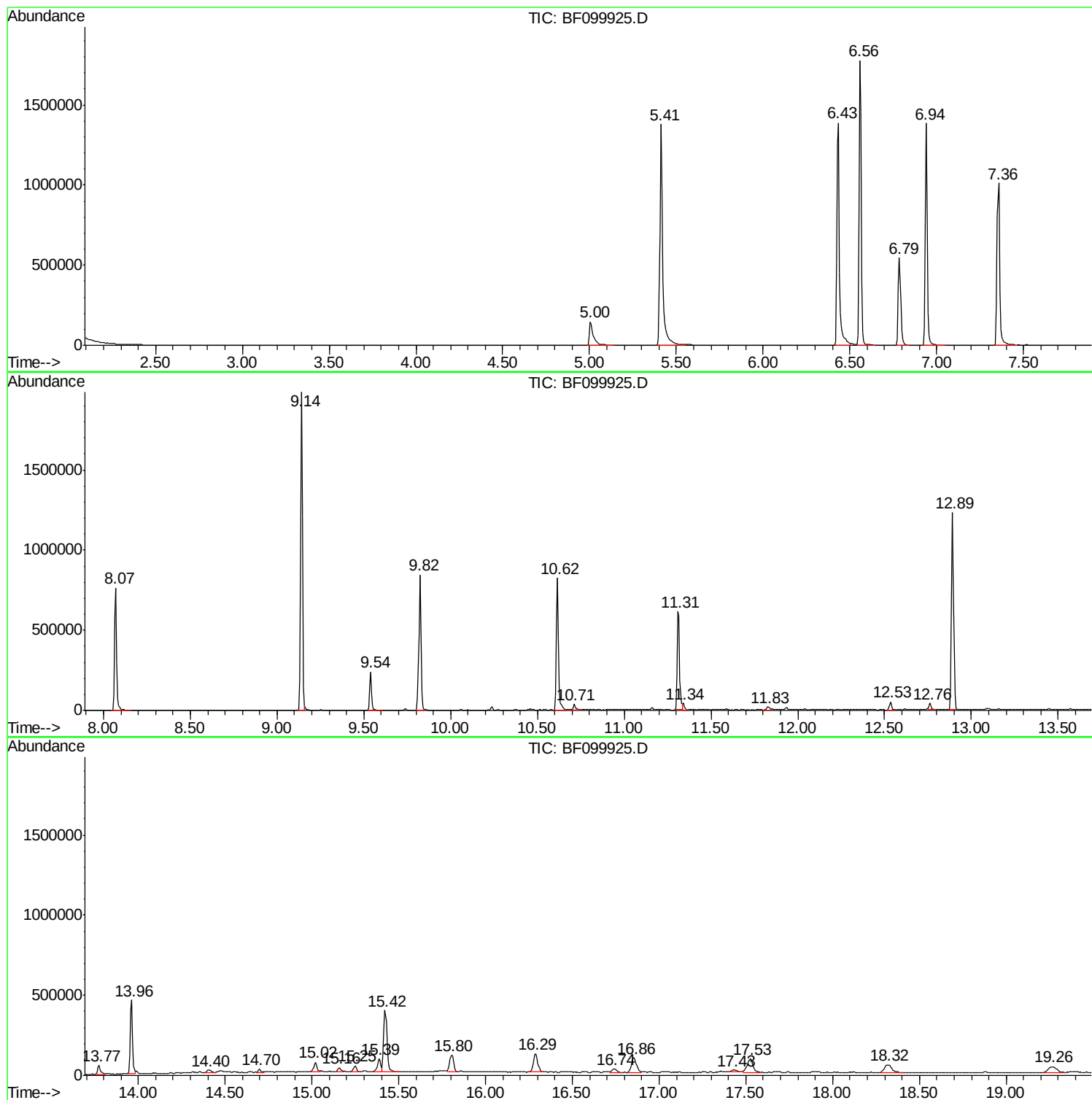
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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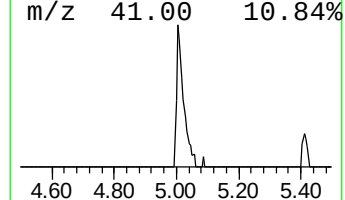
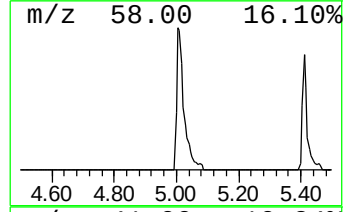
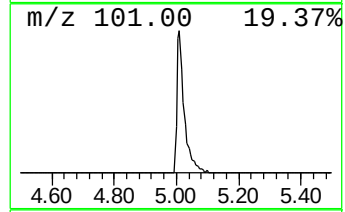
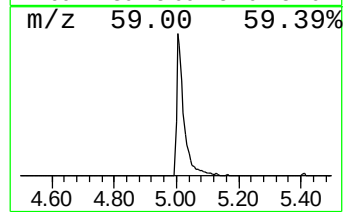
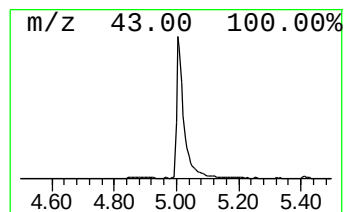
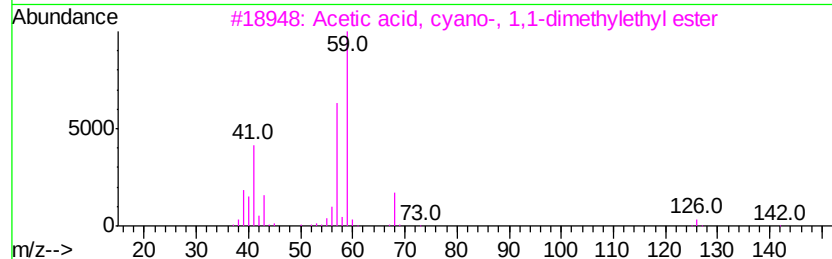
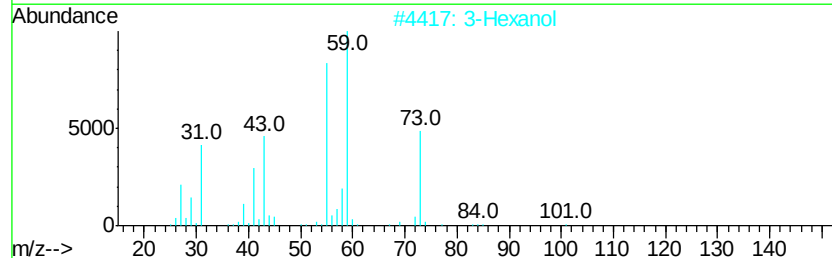
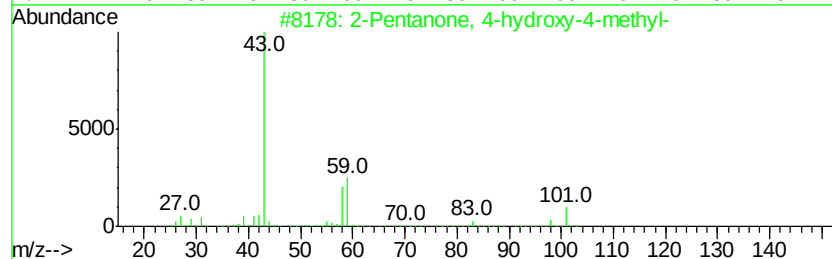
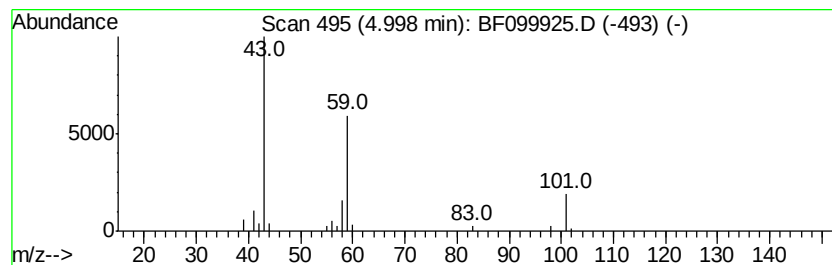
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	9.73 ng	236424	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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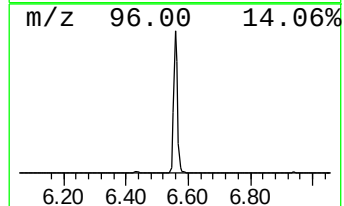
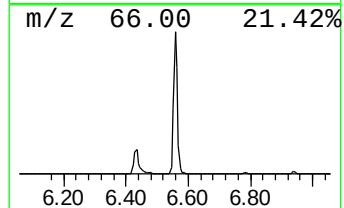
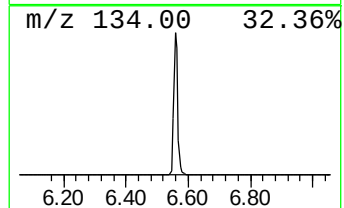
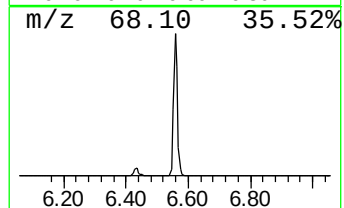
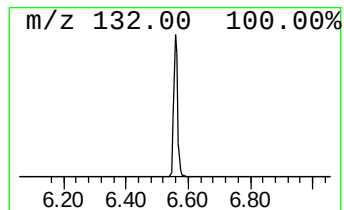
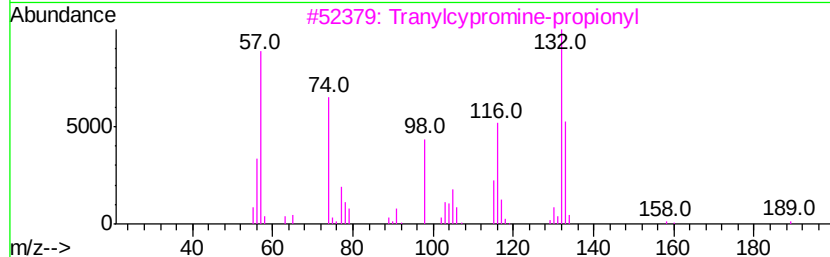
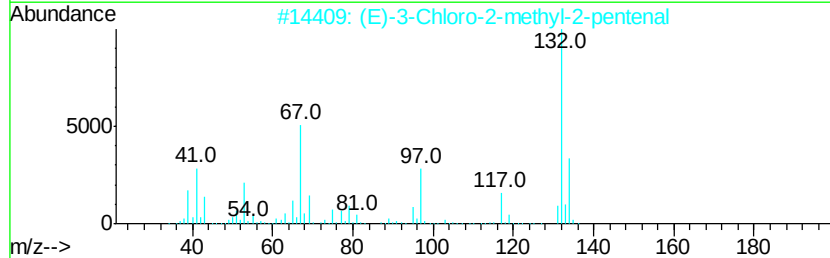
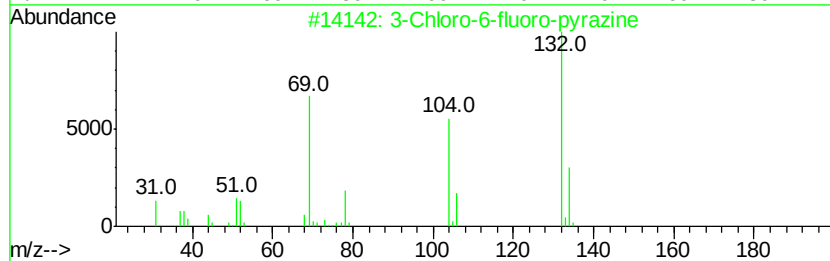
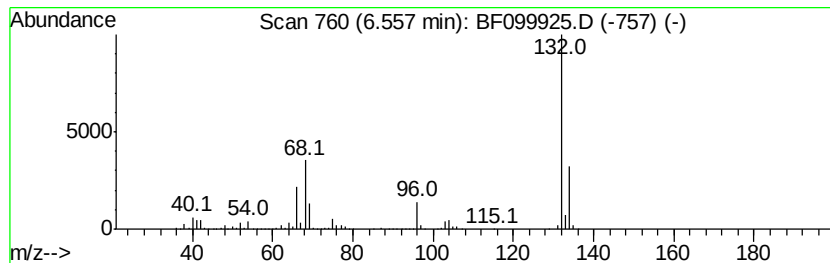
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	66.97 ng	1626630	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
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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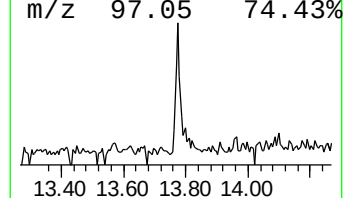
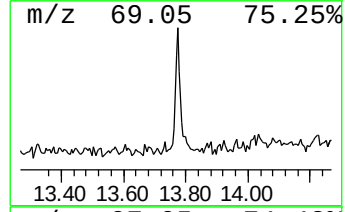
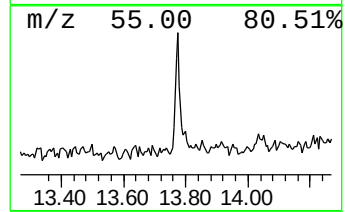
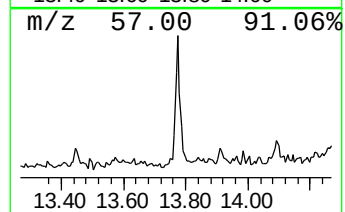
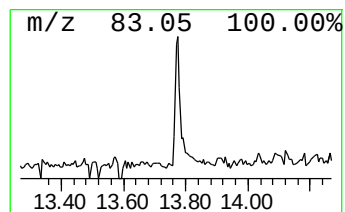
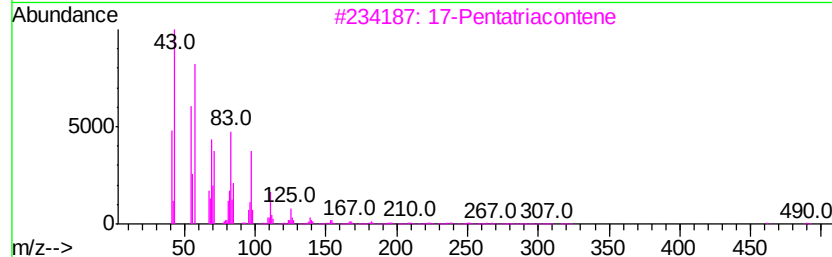
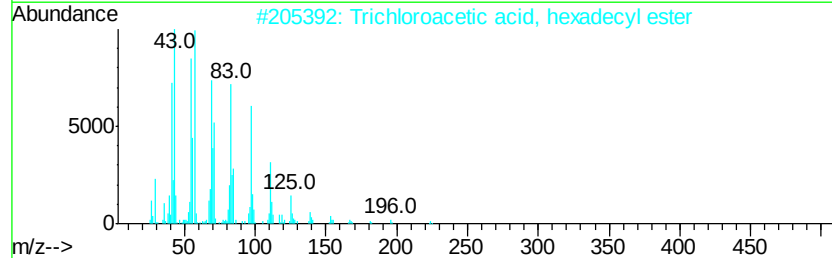
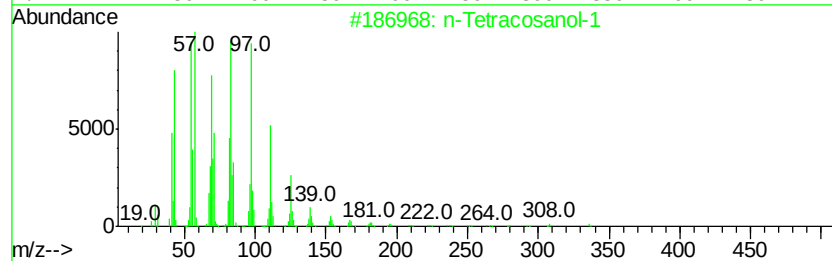
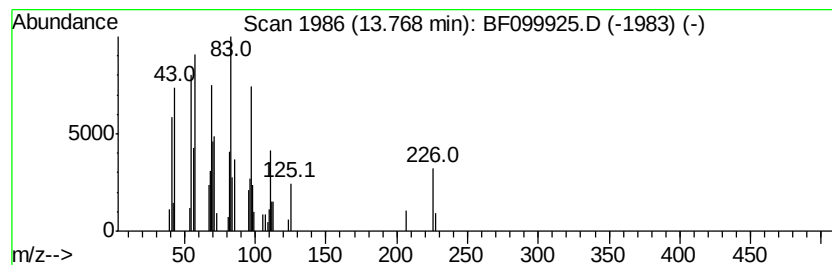
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.80 ng	61364	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Tetracosanol-1	354 C24H50O	000506-51-4 94
2		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 91
3		17-Pentatriacontene	491 C35H70	006971-40-0 91
4		2- Chloropropionic acid, octadec...	360 C21H41ClO2	088104-31-8 91
5		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 91



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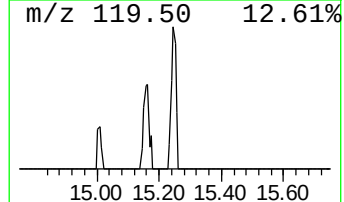
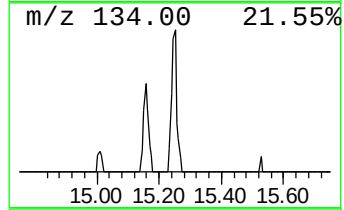
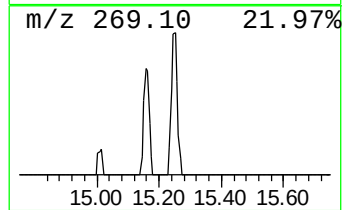
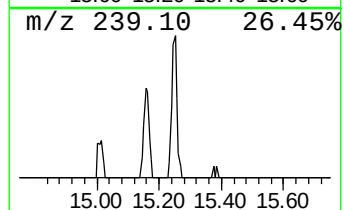
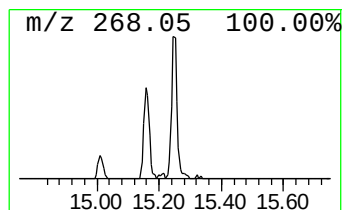
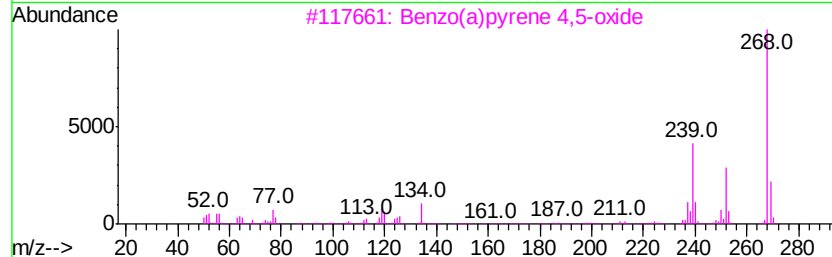
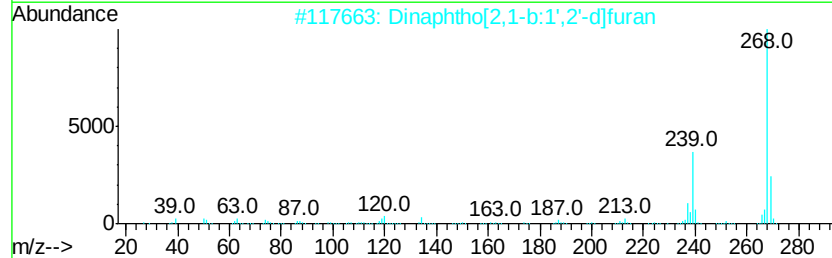
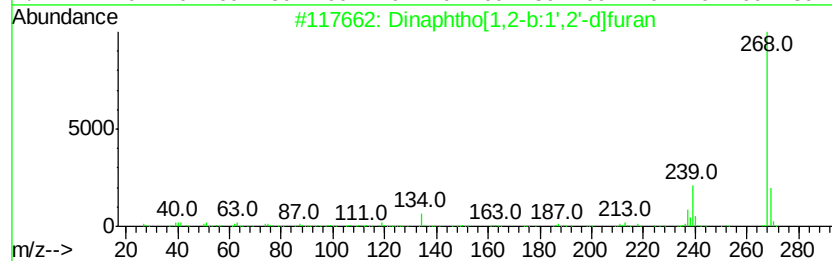
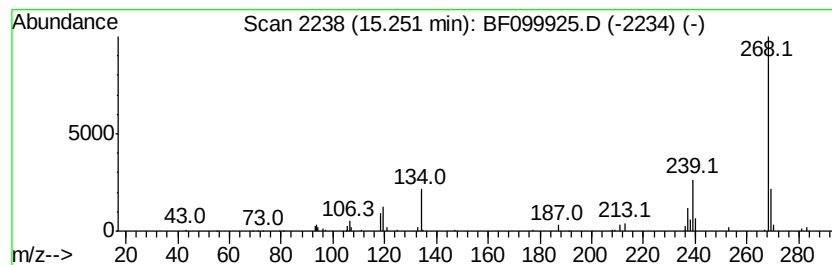
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dinaphtho[1,2-b:1',2'-d]furan Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.05 ng	48373	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	93
2		Dinaphtho[2,1-b:1',2'-d]furan	268	C20H12O	000194-63-8	83
3		Benzo(a)pyrene 4,5-oxide	268	C20H12O	037574-47-3	80
4		9,10-Anthracenedione, 1,5-dimeth...	268	C16H12O4	006448-90-4	59
5		Benzo(a)pyren-7-ol	268	C20H12O	037994-82-4	59



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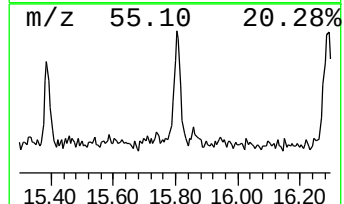
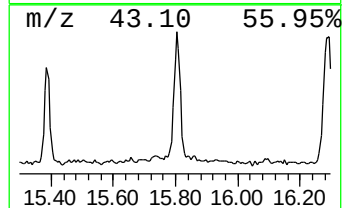
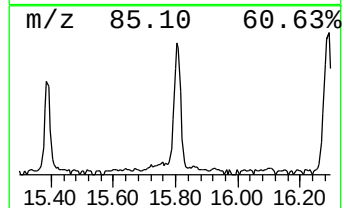
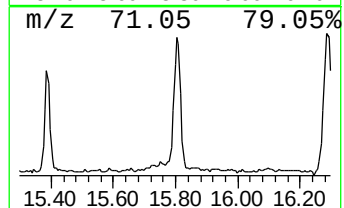
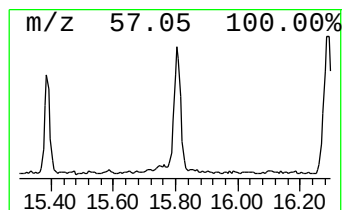
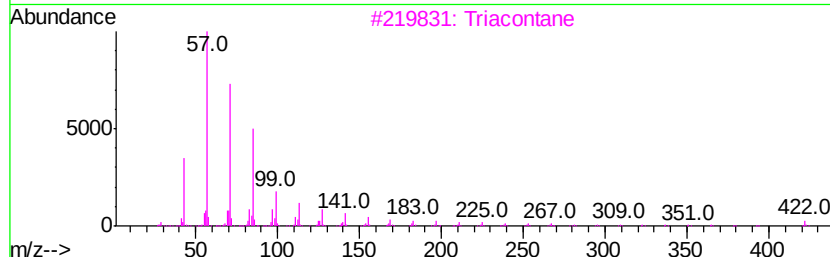
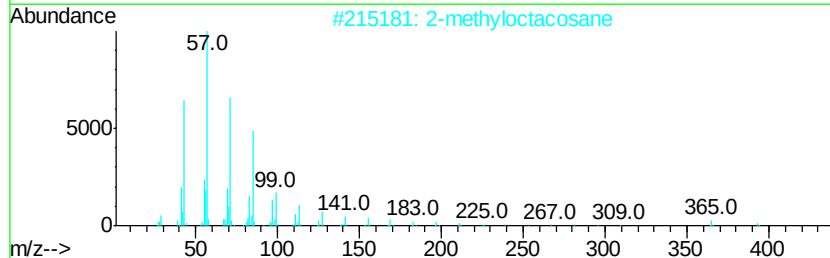
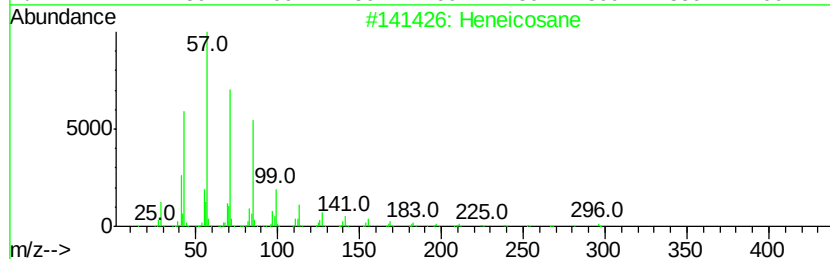
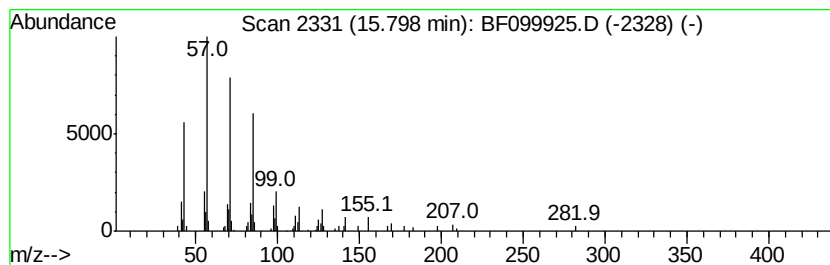
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	6.31 ng	148923	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Triacotane	422	C30H62	000638-68-6	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Hexacosane	366	C26H54	000630-01-3	91



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ClientSampleId :
SP-1-B-COMP

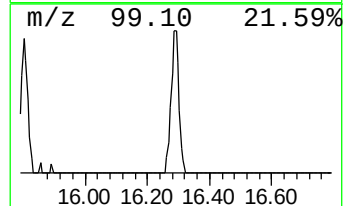
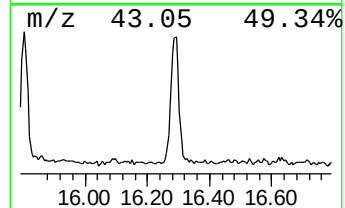
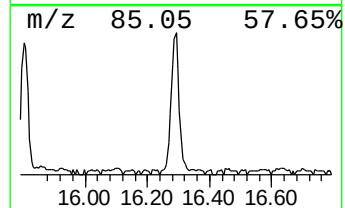
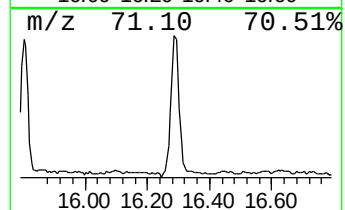
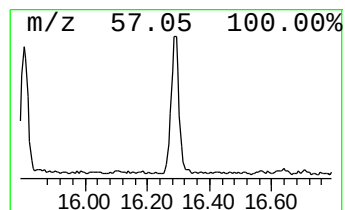
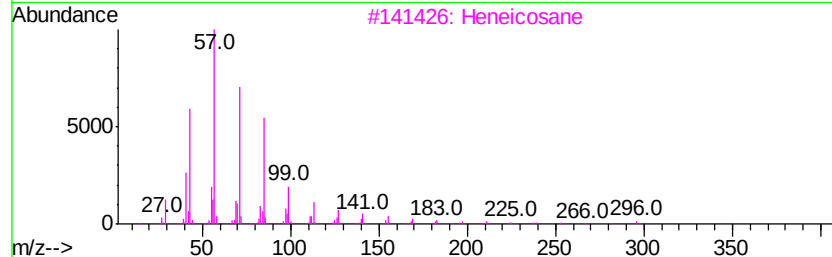
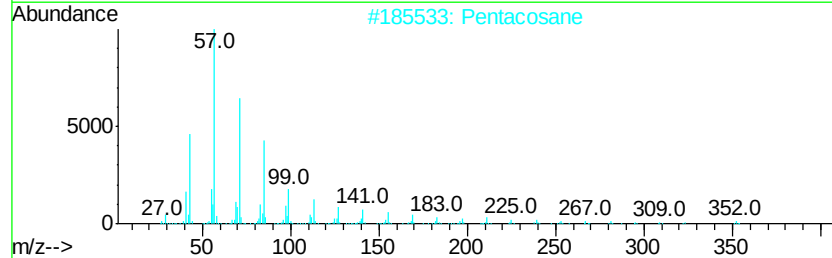
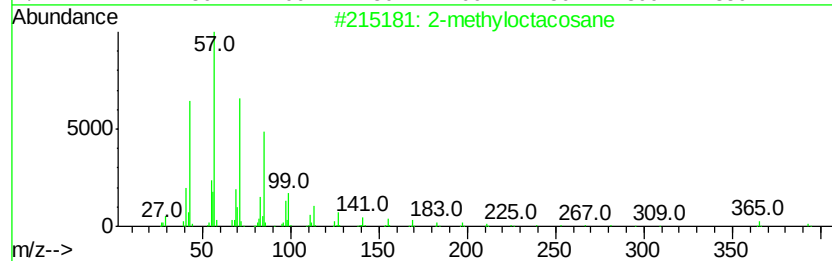
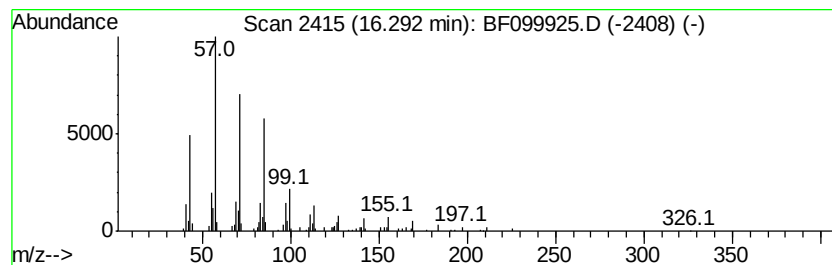
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	8.84 ng	208604	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099925.D
Acq On : 28 Oct 2017 18:54
Operator : SJ/JU
Sample : I6141-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-B-COMP

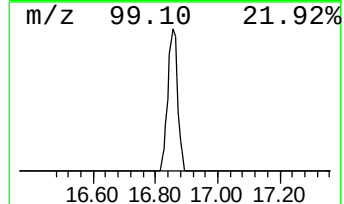
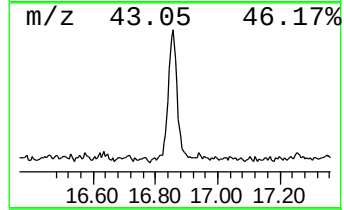
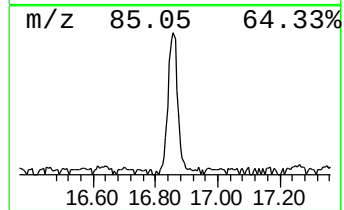
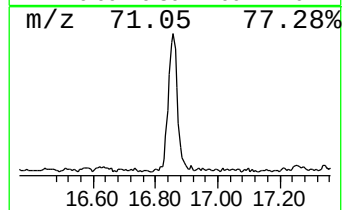
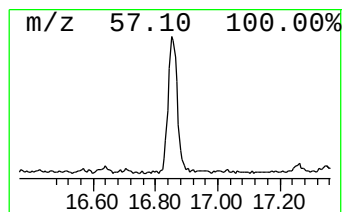
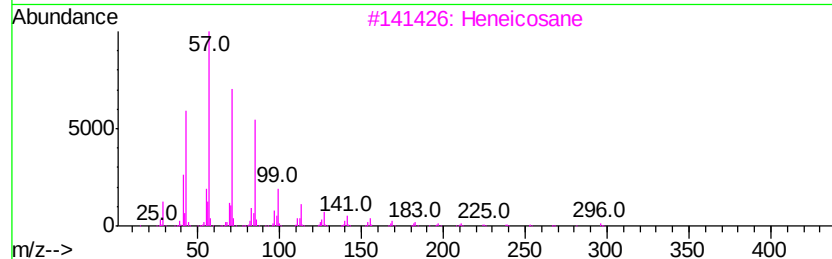
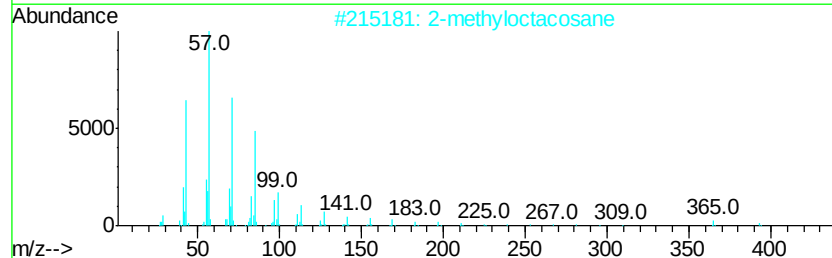
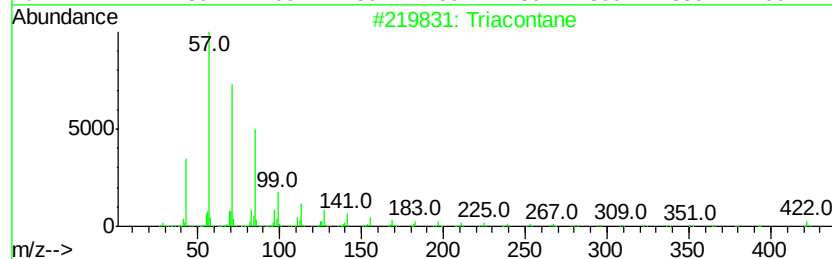
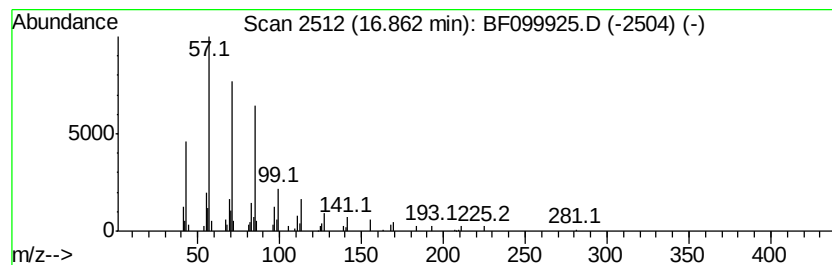
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	7.86 ng	185399	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099925.D
Acq On : 28 Oct 2017 18:54
Operator : SJ/JU
Sample : I6141-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-B-COMP

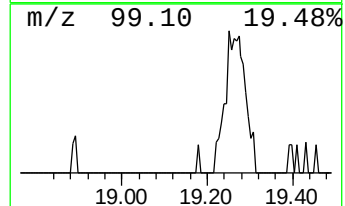
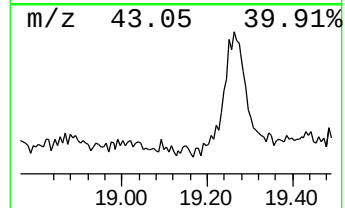
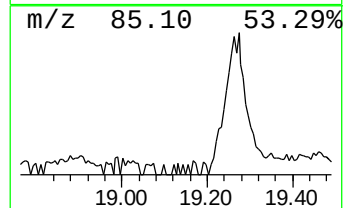
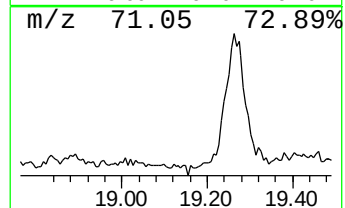
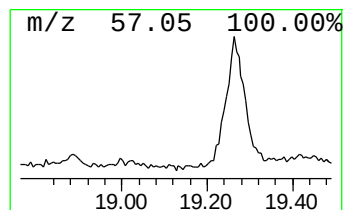
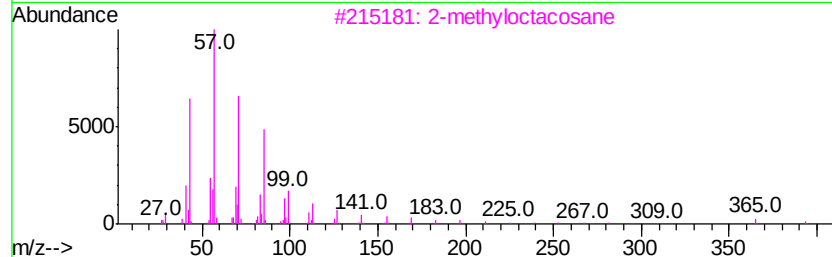
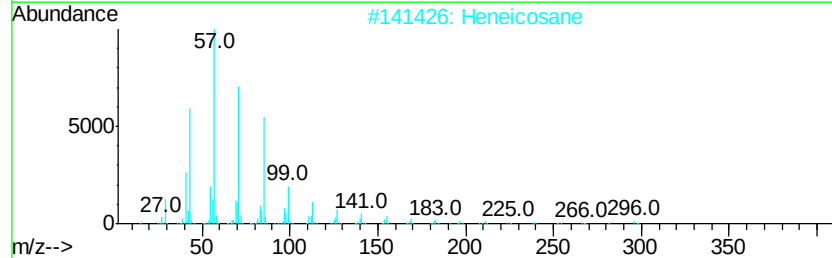
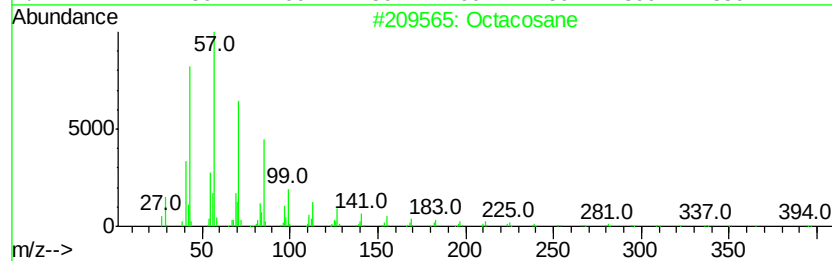
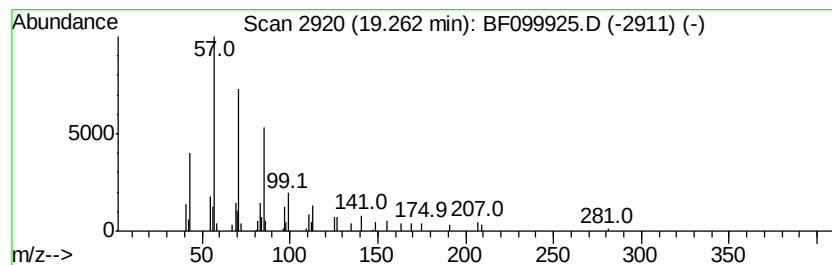
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	5.44 ng	128469	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heneicosane	296	C21H44	000629-94-7	87
3		2-methyloctacosane	408	C29H60	1000376-72-8	83
4		Hentriacontane	437	C31H64	000630-04-6	83
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099925.D
Acq On : 28 Oct 2017 18:54
Operator : SJ/JU
Sample : I6141-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
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unknown6.56	6.56	67.0	ng	1626630	1	6.79	485790	20.0
n-Tetracosanol-1	13.77	2.8	ng	61364	5	13.96	439015	20.0
Dinaphtho[1,2-b:1...	15.25	2.0	ng	48373	6	15.42	471965	20.0
Heneicosane	15.80	6.3	ng	148923	6	15.42	471965	20.0
2-methyloctacosane	16.29	8.8	ng	208604	6	15.42	471965	20.0
Triacontane	16.86	7.9	ng	185399	6	15.42	471965	20.0
Octacosane	19.26	5.4	ng	128469	6	15.42	471965	20.0