

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071117\  
 Data File : BF096662.D  
 Acq On : 12 Jul 2017 00:30  
 Operator : SJ/JU  
 Sample : PB100552BL  
 Misc :  
 ALS Vial : 27 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB100552BL

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-BF070117.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	4.881	470	475	490	rBV	476660	672728	21.64%	2.603%
2	5.304	542	547	550	rBV	2948545	2978066	95.80%	11.522%
3	6.328	715	721	724	rBV	2888874	3054785	98.26%	11.819%
4	6.457	738	743	746	rBV	2984708	2923966	94.06%	11.313%
5	6.681	778	781	785	rBV	818153	695357	22.37%	2.690%
6	6.839	804	808	812	rBV	2454639	2285789	73.53%	8.843%
7	7.245	872	877	880	rBV	1821691	1911519	61.49%	7.395%
8	7.963	995	999	1003	rBV	1021011	933065	30.01%	3.610%
9	9.045	1177	1183	1186	rBV	2951960	3108782	100.00%	12.028%
10	9.716	1291	1297	1301	rBV	1045969	898315	28.90%	3.475%
11	10.504	1425	1431	1434	rBV	1487683	1553149	49.96%	6.009%
12	11.192	1544	1548	1552	rBV	1009250	869919	27.98%	3.366%
13	12.780	1813	1818	1821	rBV	2304853	2394326	77.02%	9.263%
14	13.821	1991	1995	2002	rVB	764340	707726	22.77%	2.738%
15	15.221	2227	2233	2237	rBV	447057	552071	17.76%	2.136%
16	15.268	2238	2241	2248	rVB2	40133	51930	1.67%	0.201%
17	15.668	2304	2309	2314	rBV	38310	59041	1.90%	0.228%
18	16.127	2382	2387	2394	rBV	39041	66557	2.14%	0.258%
19	16.662	2473	2478	2485	rVB3	33306	65042	2.09%	0.252%
20	17.298	2581	2586	2595	rVB3	26419	64981	2.09%	0.251%

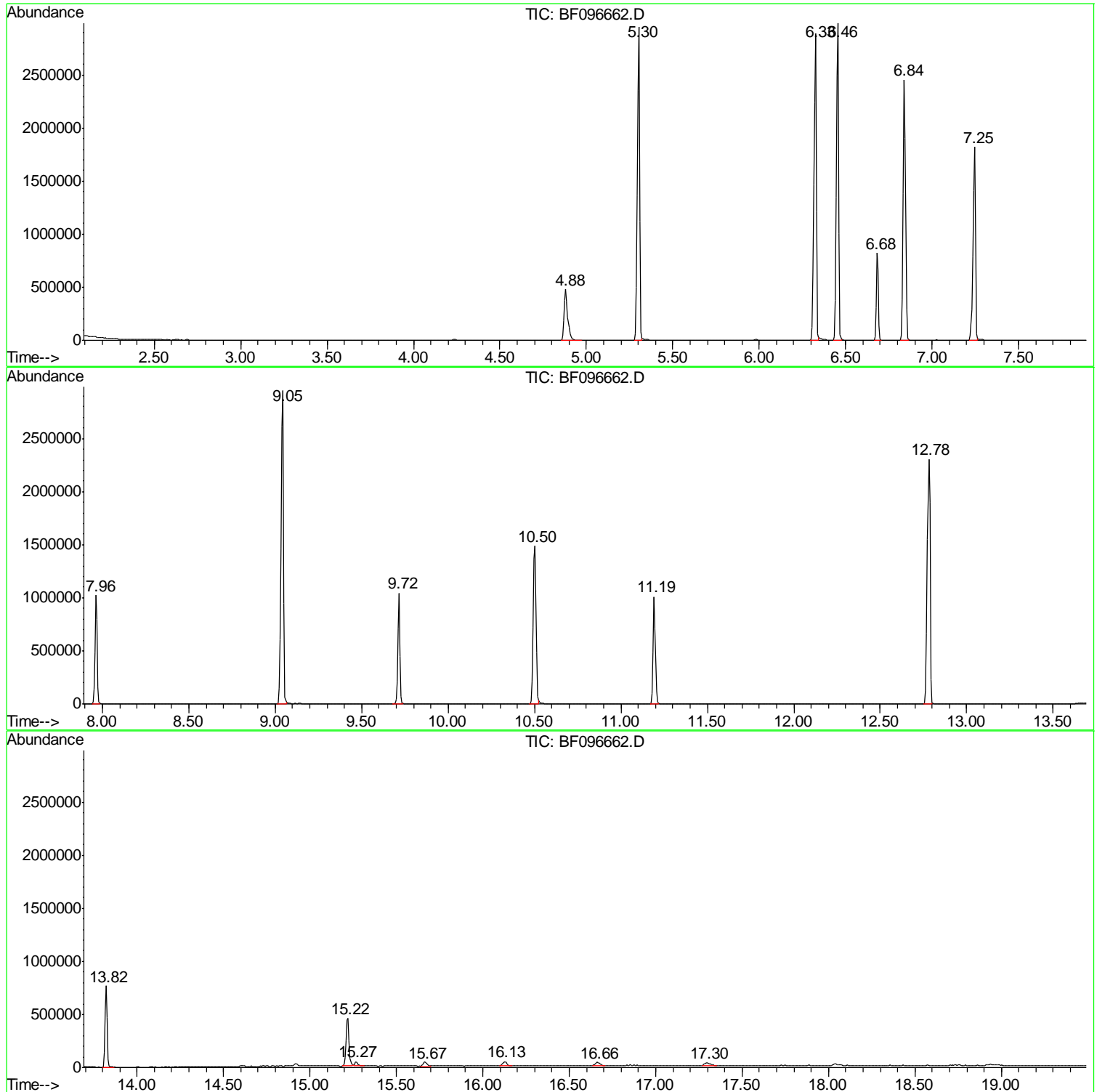
Sum of corrected areas: 25847114

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ALS Vial : 27 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampled :  
PB100552BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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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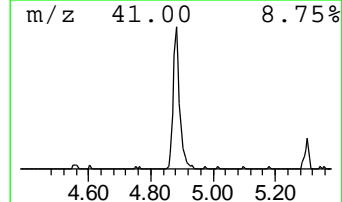
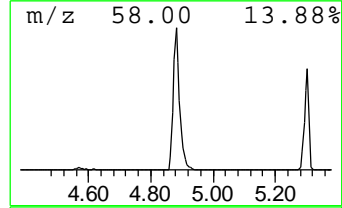
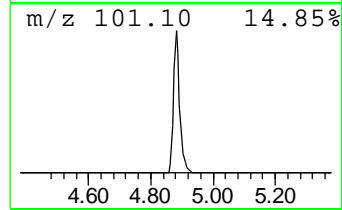
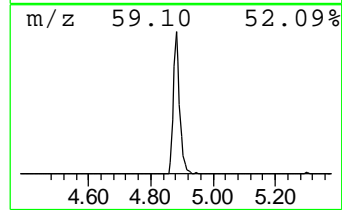
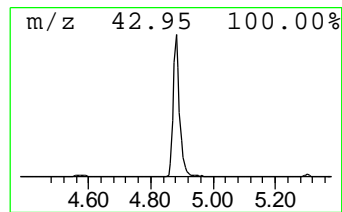
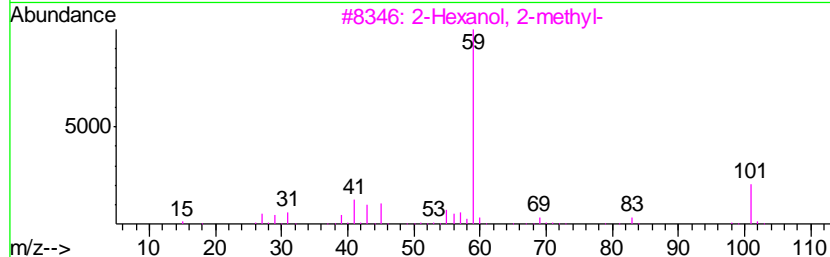
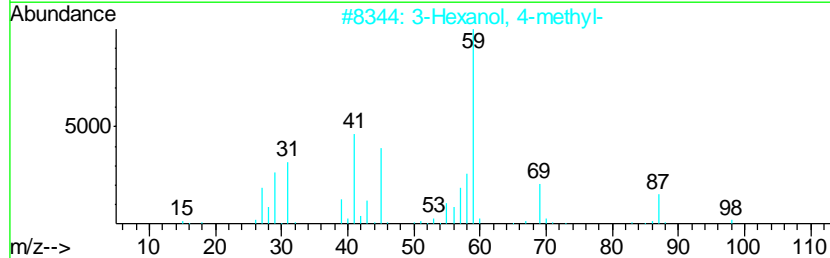
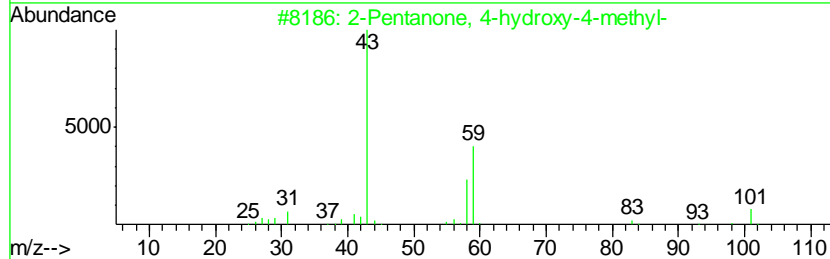
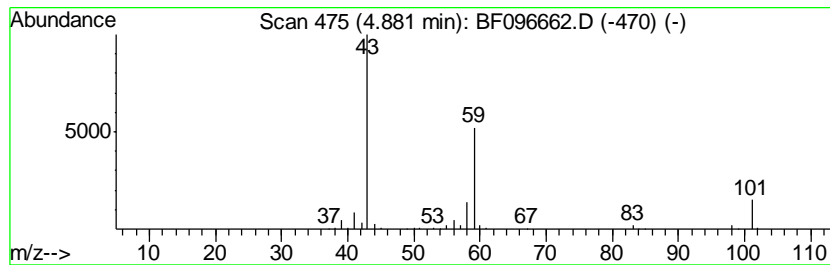
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	19.35 ng	672728	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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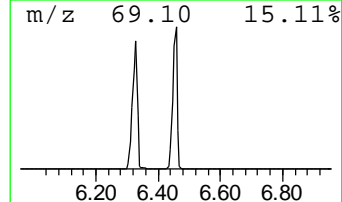
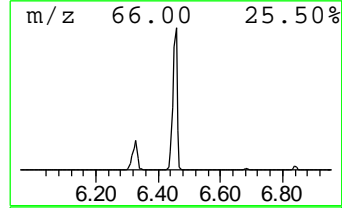
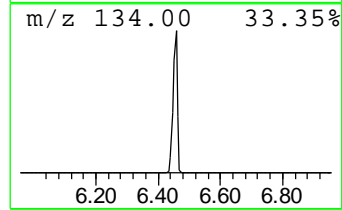
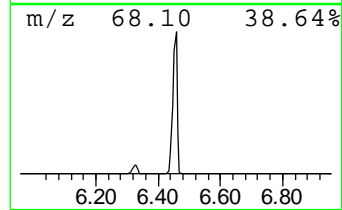
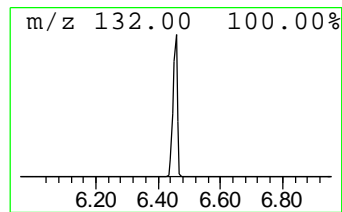
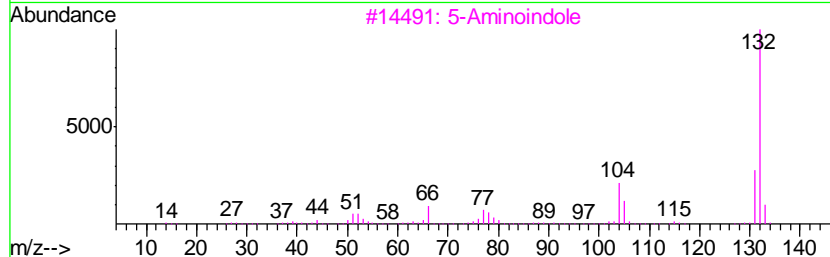
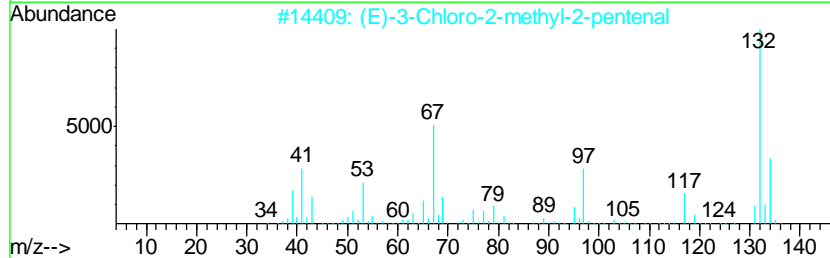
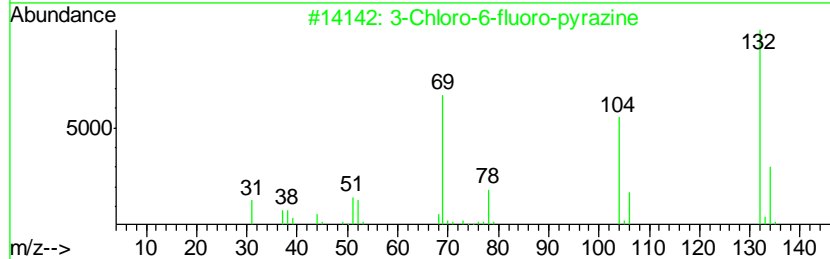
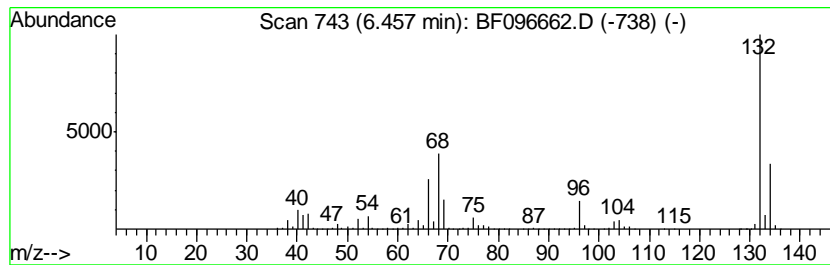
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	84.10 ng	2923970	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
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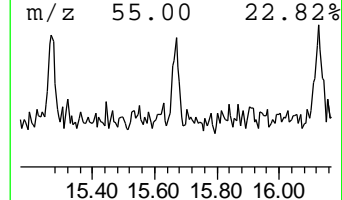
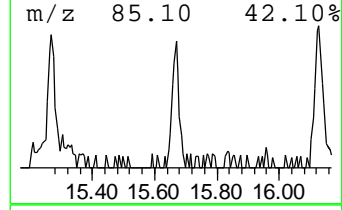
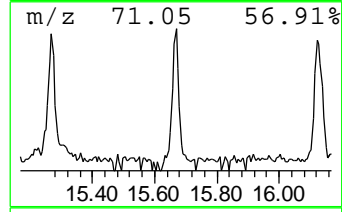
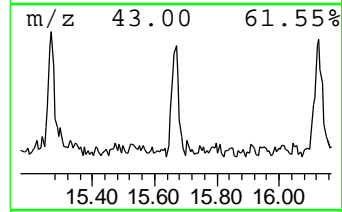
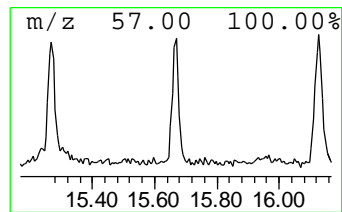
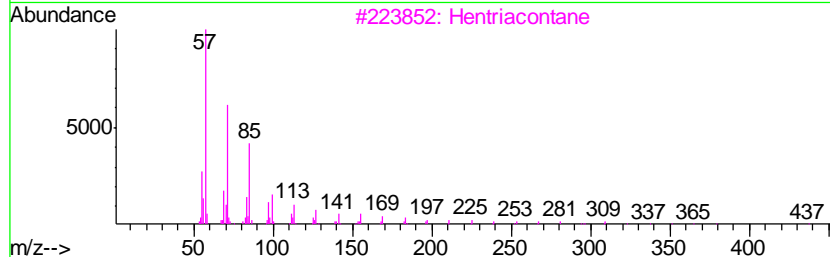
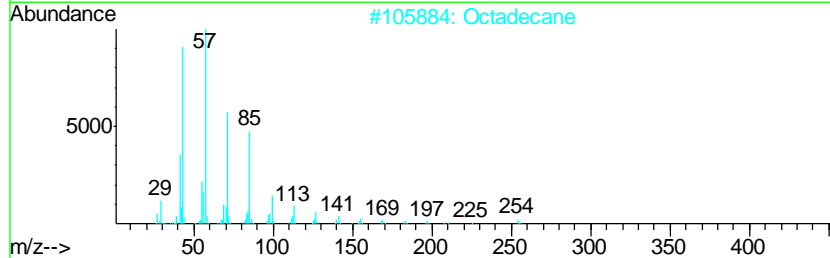
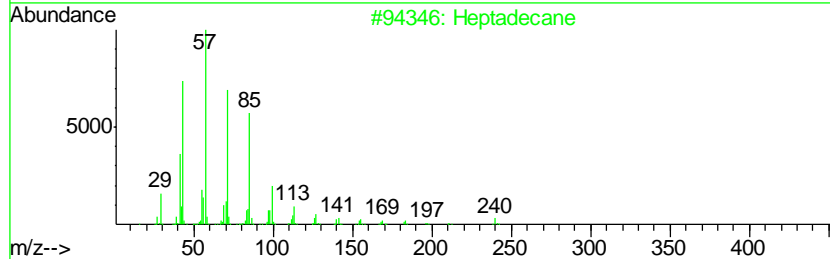
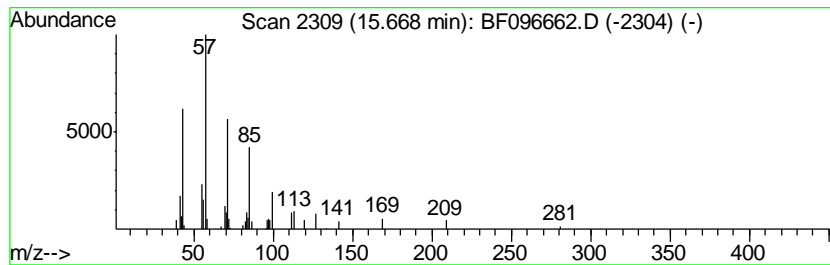
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.14 ng	59041	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	87
2		Octadecane	254	C18H38	000593-45-3	86
3		Hentriacontane	437	C31H64	000630-04-6	86
4		Tetracosane	338	C24H50	000646-31-1	83
5		Heneicosane	296	C21H44	000629-94-7	83



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 Misc :  
 ALS Vial : 27 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampled :  
 PB100552BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

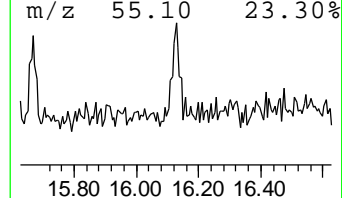
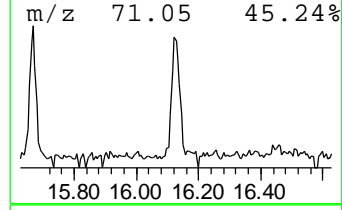
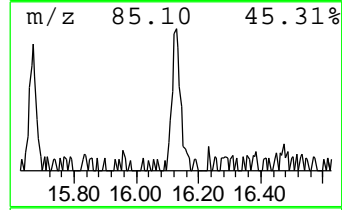
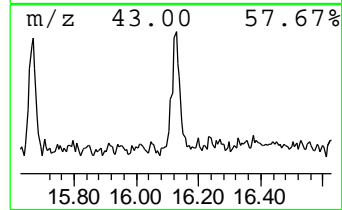
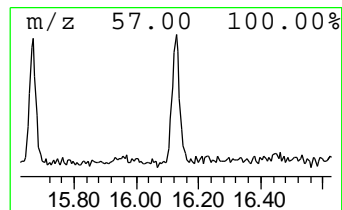
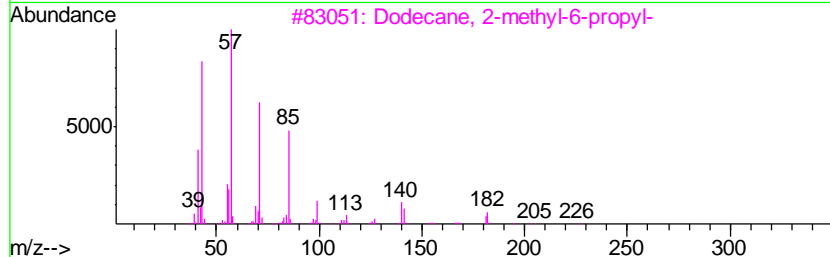
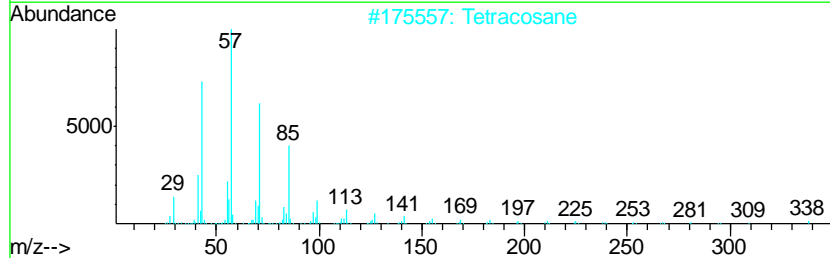
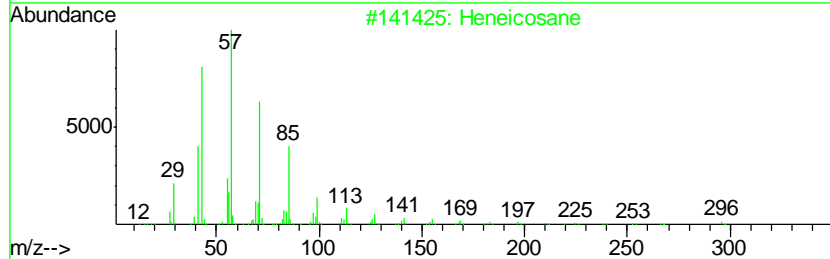
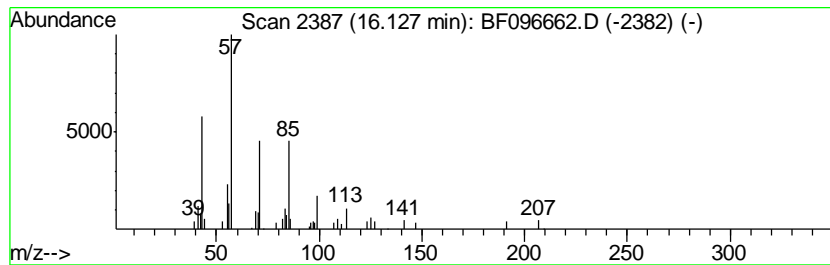
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.41 ng	66557	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	64
2		Tetracosane	338	C24H50	000646-31-1	64
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
4		Heptadecane	240	C17H36	000629-78-7	59
5		Tridecane, 6-propyl-	226	C16H34	055045-10-8	53



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 PB100552BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
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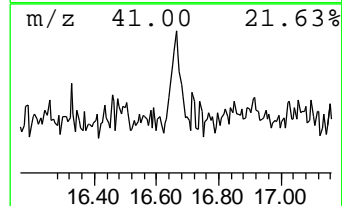
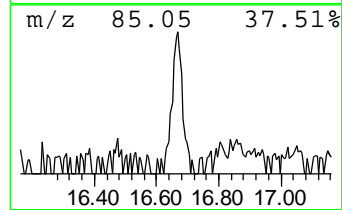
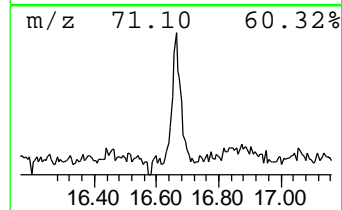
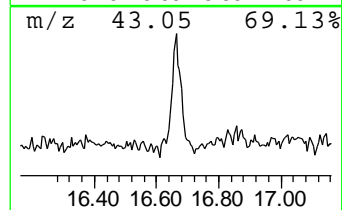
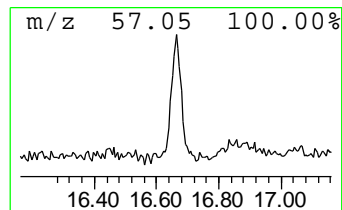
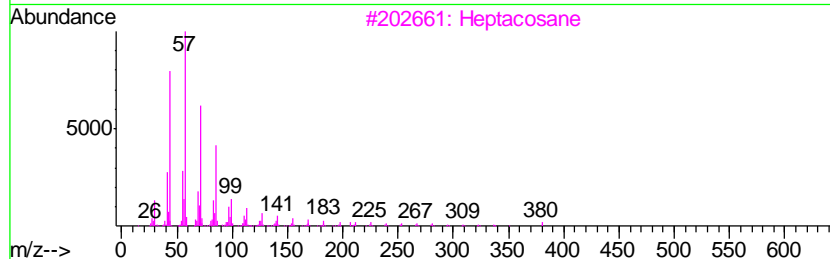
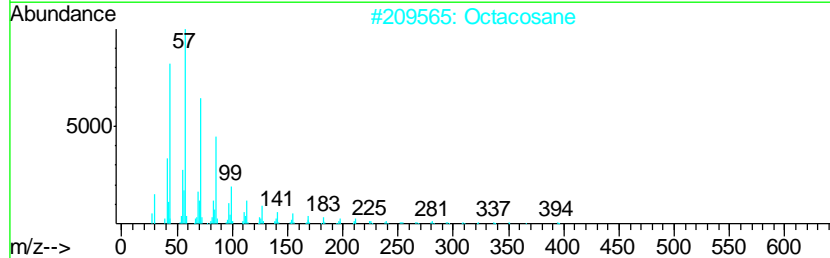
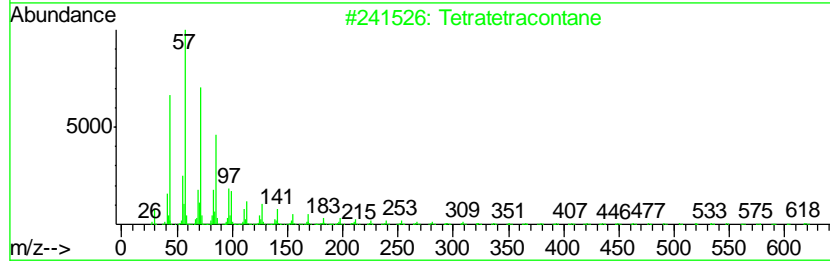
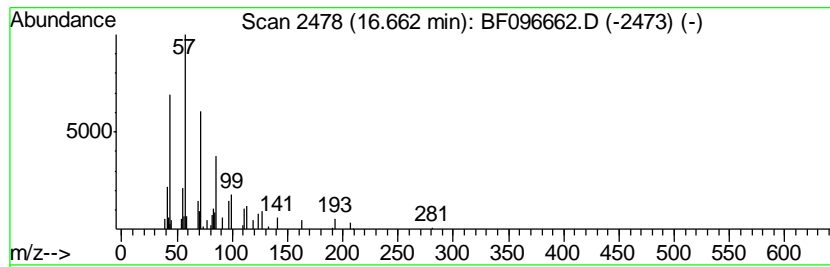
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.36 ng	65042	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Octacosane	394	C28H58	000630-02-4	86
3		Heptacosane	380	C27H56	000593-49-7	86
4		Hexatriacontane	507	C36H74	000630-06-8	86
5		Hentriacontane	437	C31H64	000630-04-6	78



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
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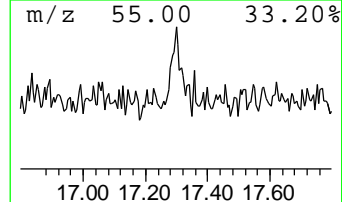
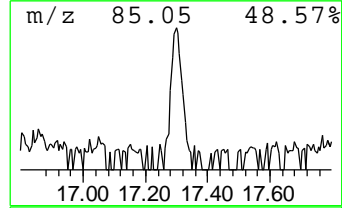
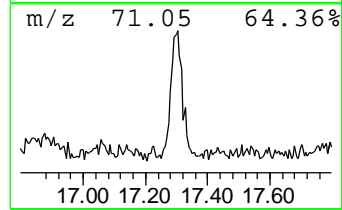
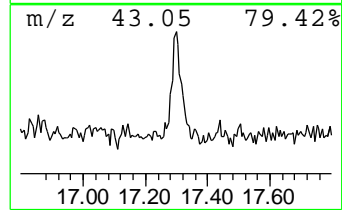
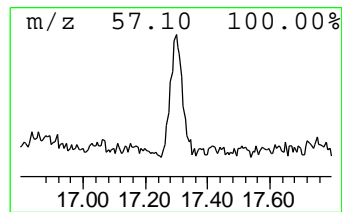
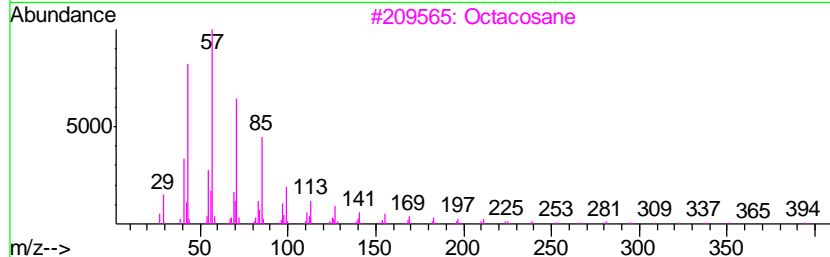
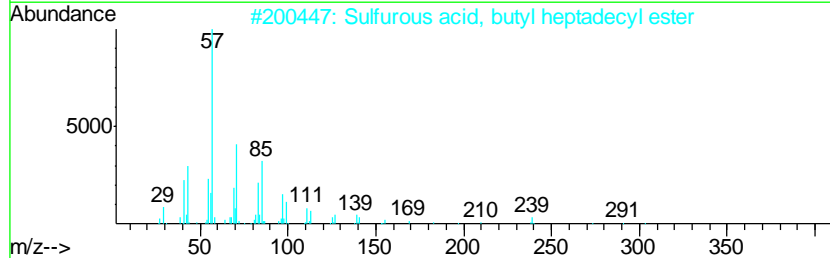
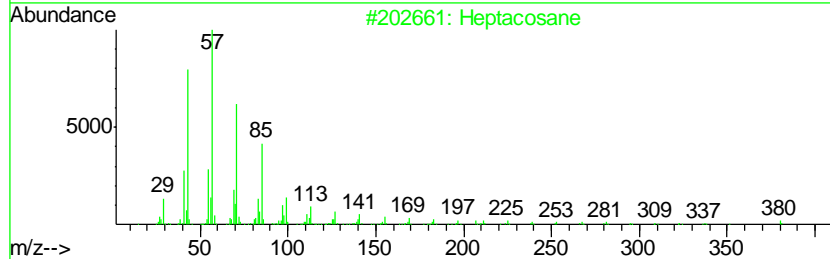
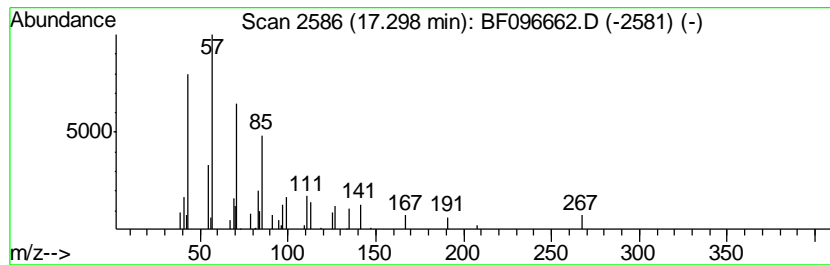
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.35 ng	64981	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	72
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72
3		Octacosane	394	C28H58	000630-02-4	64
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	64
5		Tetrapentacontane	759	C54H110	005856-66-6	64





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071117\  
 Data File : BF096662.D  
 Acq On : 12 Jul 2017 00:30  
 Operator : SJ/JU  
 Sample : PB100552BL  
 Misc :  
 ALS Vial : 27 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB100552BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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...	4.88	19.4	ng	672728	1	6.68	695357	20.0
unknown6.46	6.46	84.1	ng	2923970	1	6.68	695357	20.0
Heptadecane	15.67	2.1	ng	59041	6	15.22	552071	20.0
Heneicosane	16.13	2.4	ng	66557	6	15.22	552071	20.0
Tetratetracontane	16.66	2.4	ng	65042	6	15.22	552071	20.0
Heptacosane	17.30	2.4	ng	64981	6	15.22	552071	20.0