

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
 Data File : BF101646.D
 Acq On : 22 Dec 2017 10:16
 Operator : SJ/JU
 Sample : I7008-12
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121817-TIFR-E-U-B

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-BF121417.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	5.010	494	497	507	rBV	60810	103165	2.94%	0.472%
2	5.416	563	566	589	rBV	679360	1119357	31.89%	5.123%
3	6.440	737	740	758	rBV2	415394	838639	23.89%	3.838%
4	6.569	758	762	778	rVB	1934121	2070300	58.99%	9.475%
5	6.798	797	801	810	rBV	806079	828729	23.61%	3.793%
6	6.951	823	827	843	rBV	2848142	2696178	76.82%	12.339%
7	7.369	894	898	919	rBV	2074273	2252615	64.18%	10.309%
8	8.081	1015	1019	1036	rBV	944755	1071307	30.52%	4.903%
9	9.151	1197	1201	1211	rBV	3637538	3509814	100.00%	16.063%
10	9.834	1311	1317	1330	rVB	959362	961607	27.40%	4.401%
11	10.628	1448	1452	1465	rBV	987045	1053881	30.03%	4.823%
12	11.322	1567	1570	1579	rBV	737784	759859	21.65%	3.477%
13	12.710	1802	1806	1809	rBV	154275	131634	3.75%	0.602%
14	12.904	1835	1839	1842	rBV	2705991	2463943	70.20%	11.276%
15	13.410	1922	1925	1929	rBV	117394	103958	2.96%	0.476%
16	13.792	1985	1990	1998	rBV3	29762	62705	1.79%	0.287%
17	13.969	2017	2020	2027	rBV	812557	846554	24.12%	3.874%
18	14.704	2142	2145	2149	rBV	47182	48215	1.37%	0.221%
19	15.027	2197	2200	2204	rVB	50289	51176	1.46%	0.234%
20	15.398	2259	2263	2266	rBV	63179	80716	2.30%	0.369%
21	15.439	2266	2270	2280	rVB	447041	630295	17.96%	2.885%
22	15.815	2330	2334	2338	rVB	56689	77151	2.20%	0.353%
23	16.304	2412	2417	2424	rBV3	53610	89004	2.54%	0.407%

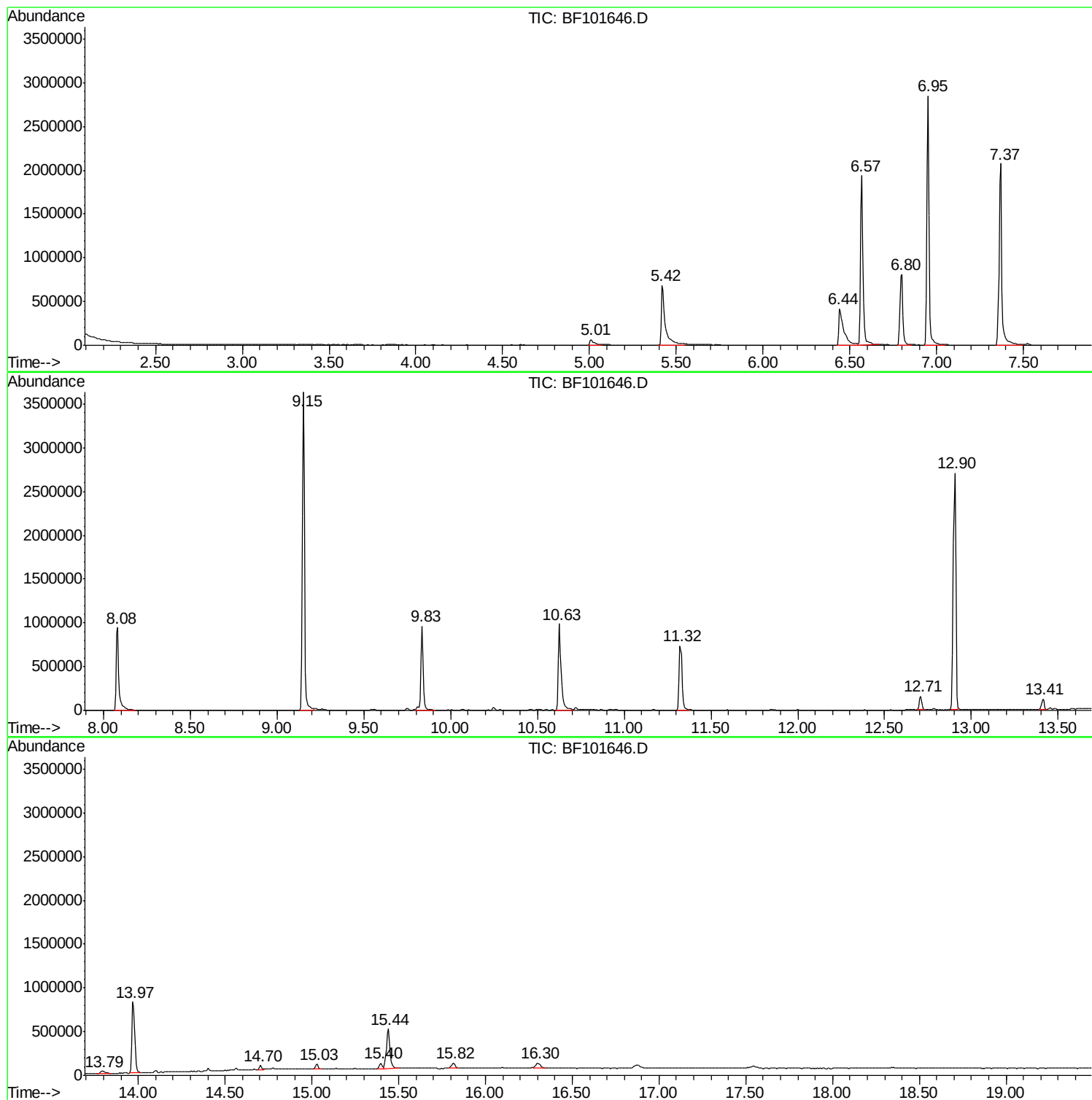
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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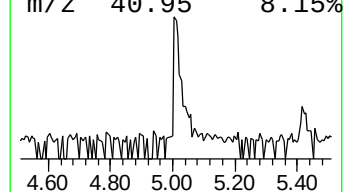
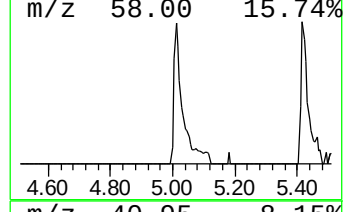
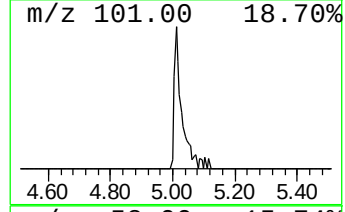
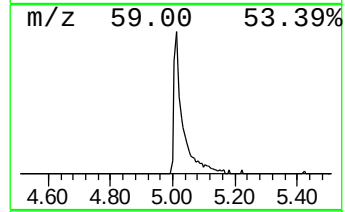
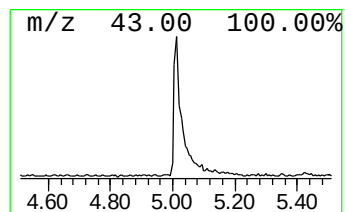
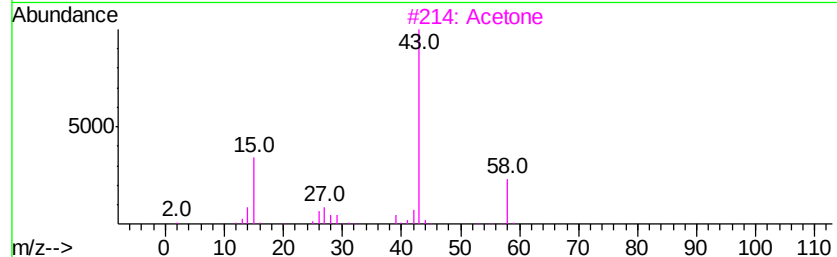
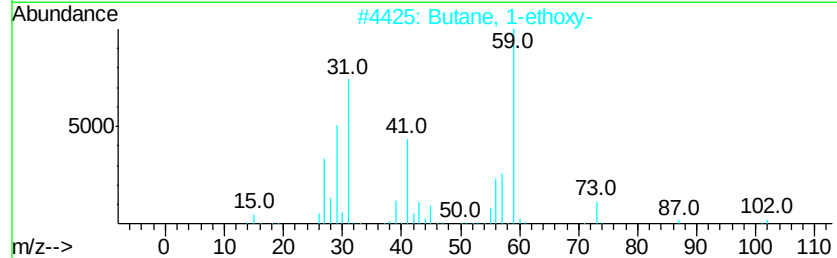
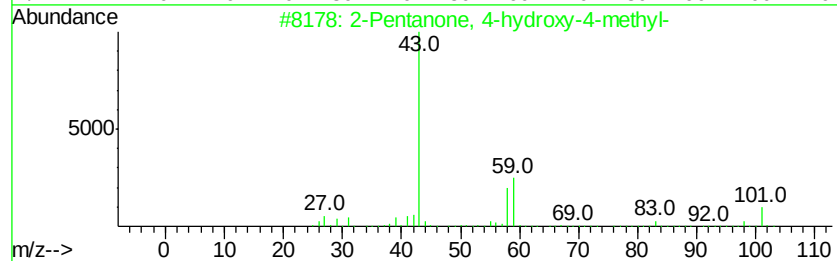
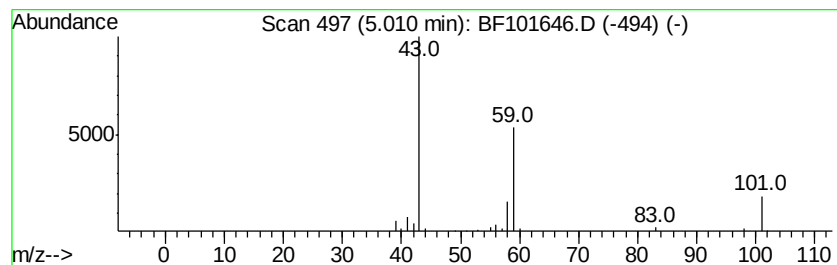
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.49 ng	103165	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3		Acetone	58	C3H6O	000067-64-1	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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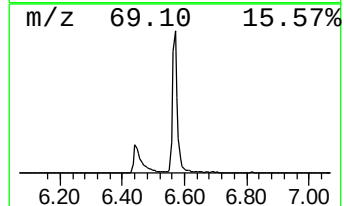
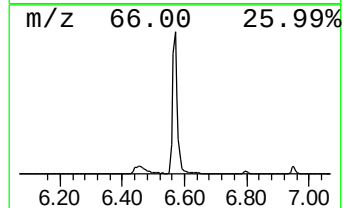
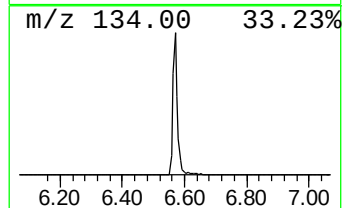
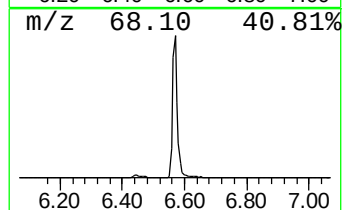
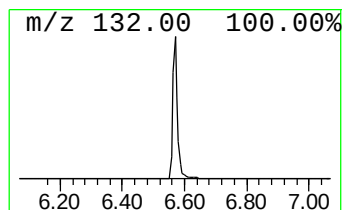
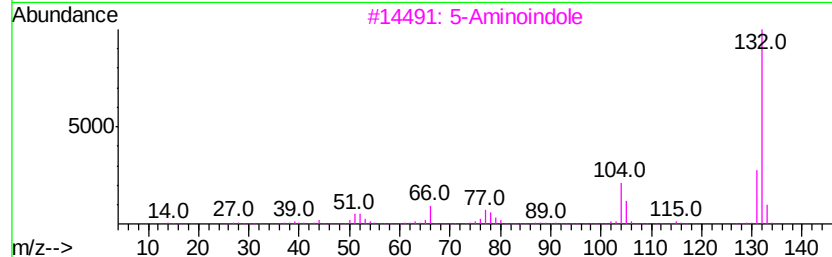
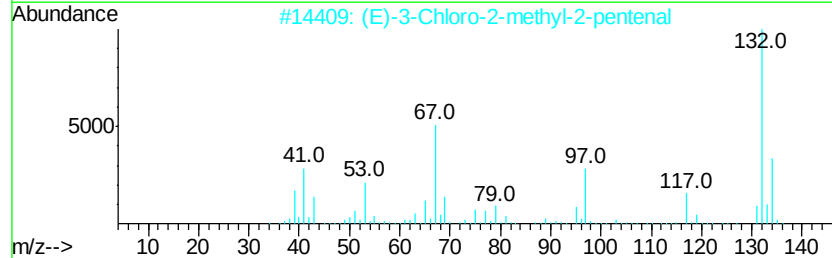
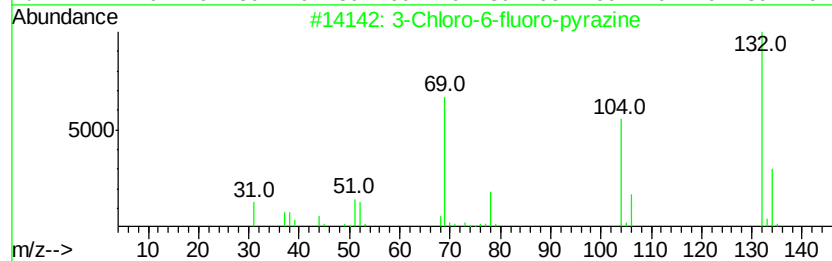
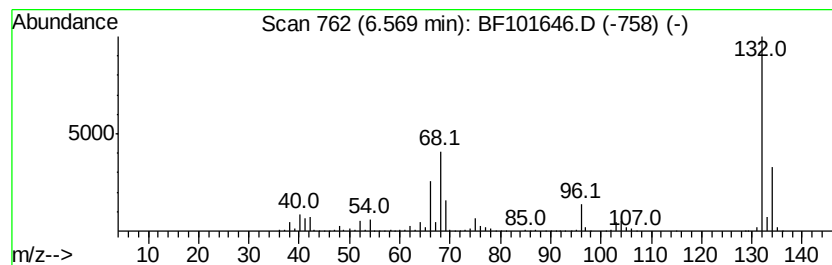
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	49.96 ng	2070300	1,4-Dichlorobenzene-d4	6.80

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	16
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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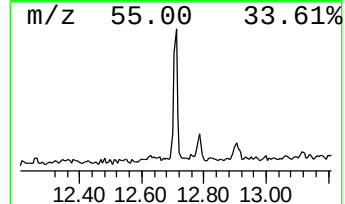
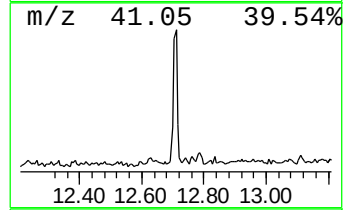
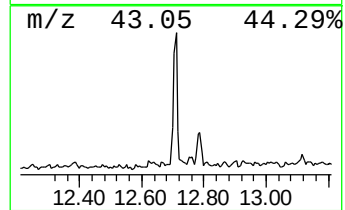
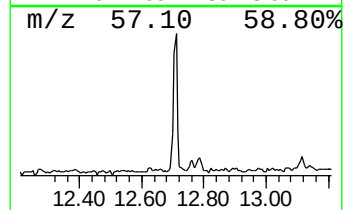
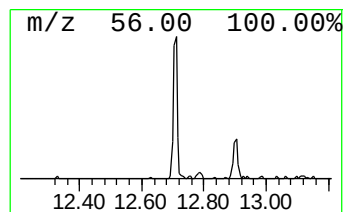
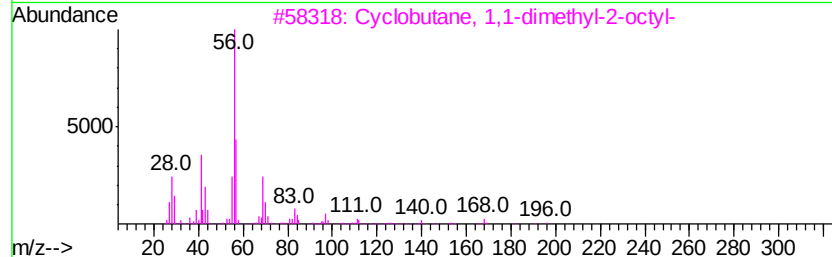
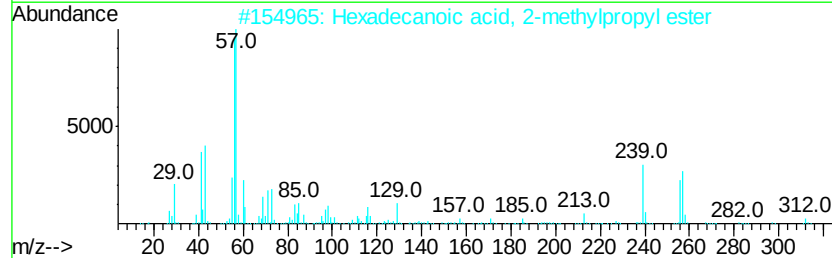
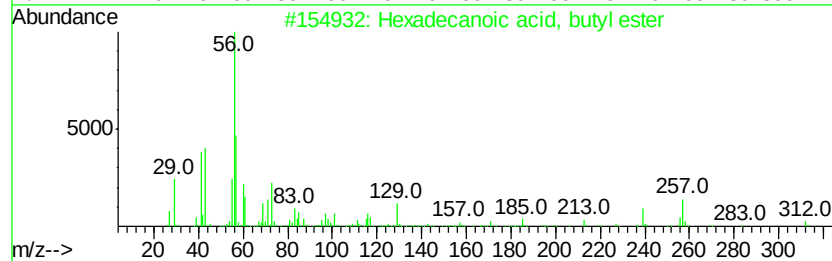
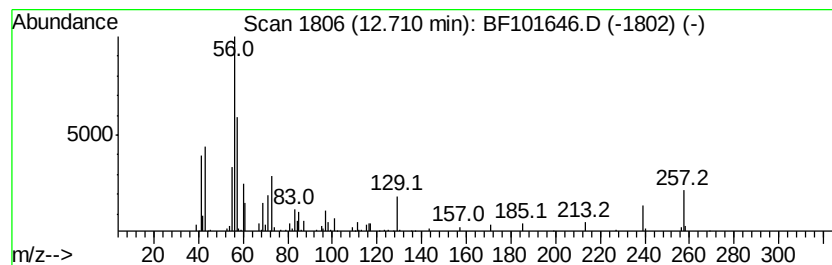
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.11 ng	131634	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2			Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	40
3			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32
5			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	27



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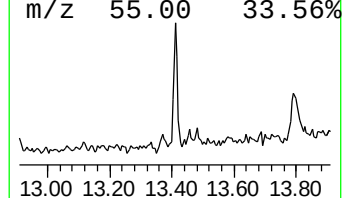
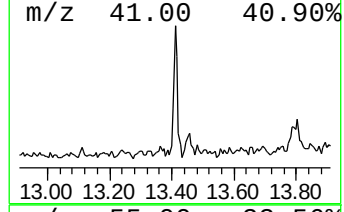
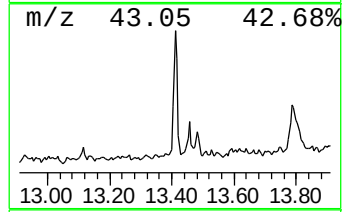
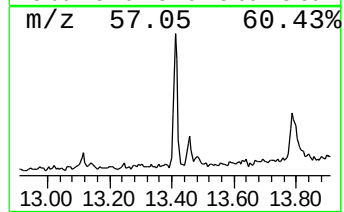
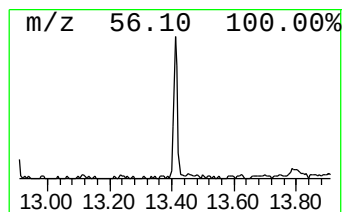
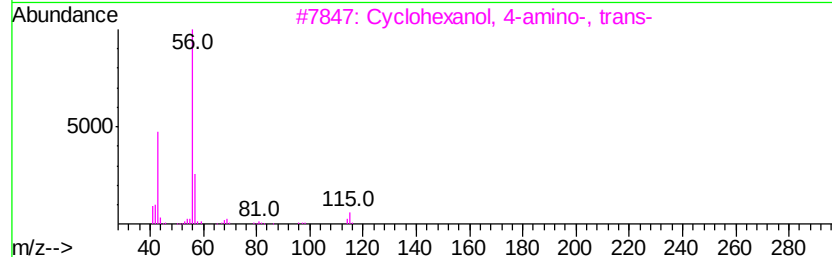
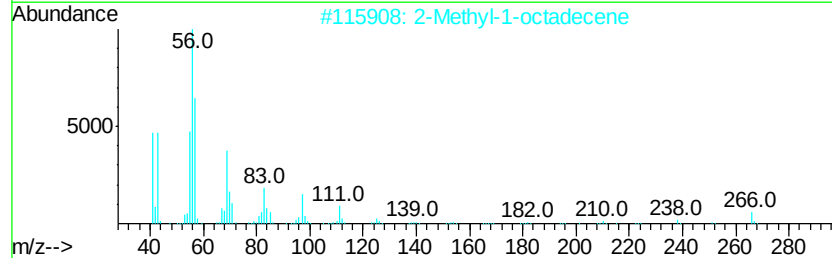
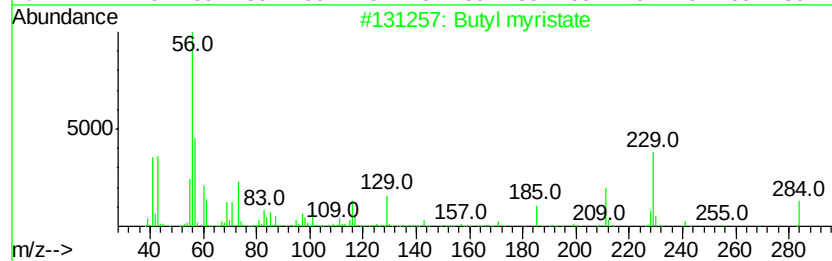
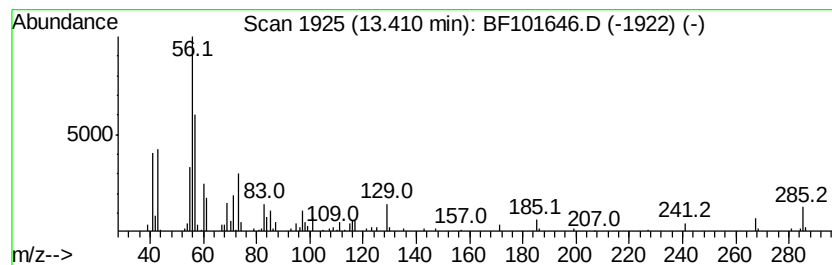
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Peak Number 5 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.41	2.46 ng	103958	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	86
2	2-Methyl-1-octadecene	266	C19H38	061868-20-0	43
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38



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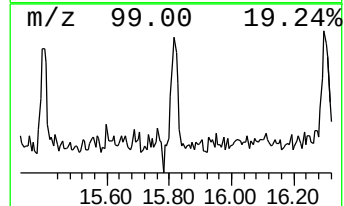
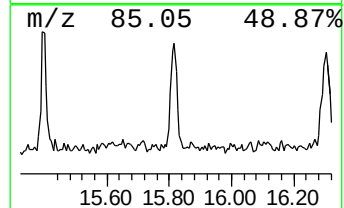
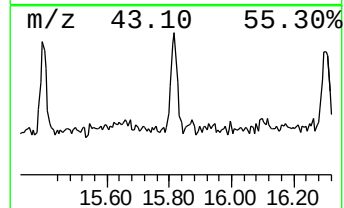
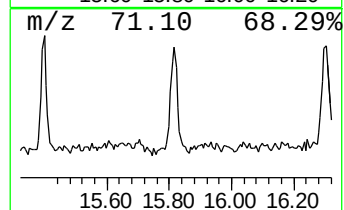
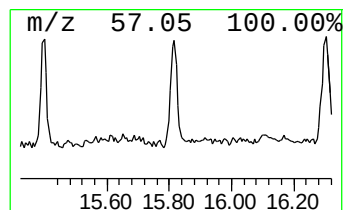
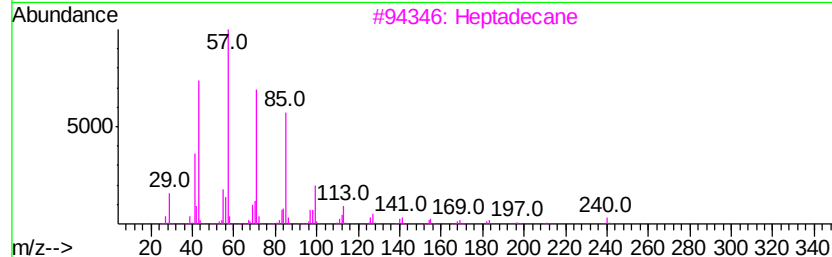
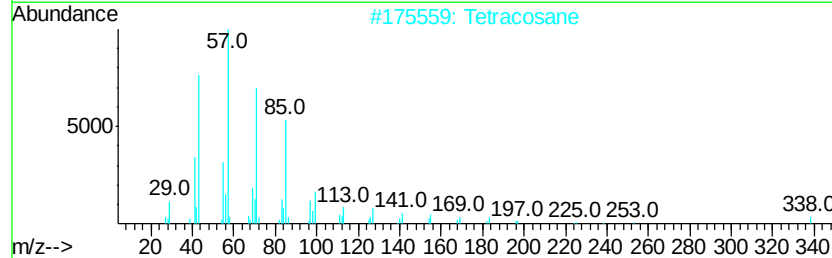
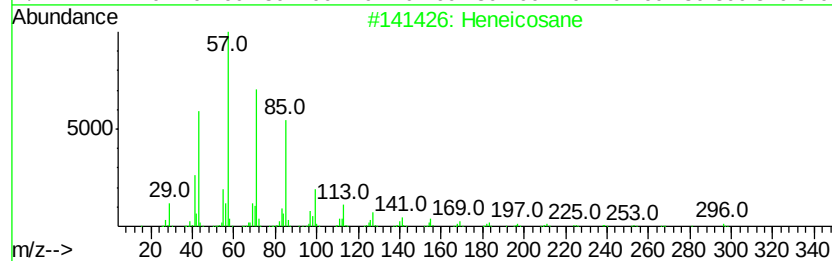
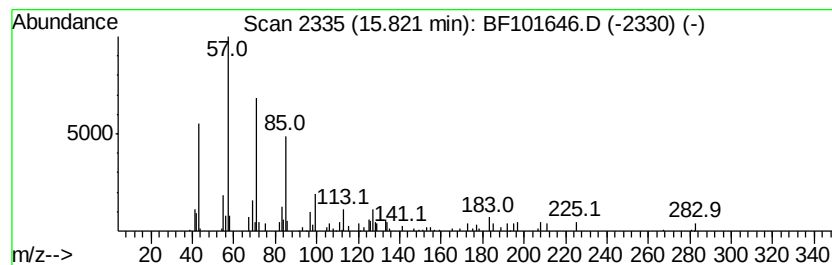
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.45 ng	77151	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Tetracosane	338	C24H50	000646-31-1	86
3		Heptadecane	240	C17H36	000629-78-7	86
4		Hexacosane	366	C26H54	000630-01-3	86
5		Octadecane	254	C18H38	000593-45-3	80



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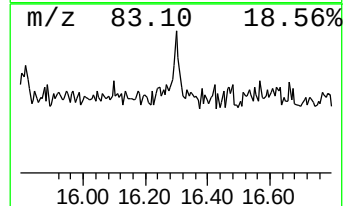
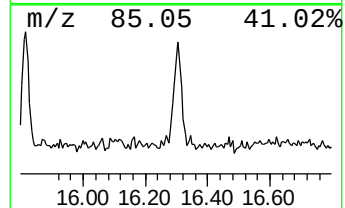
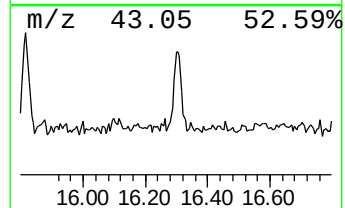
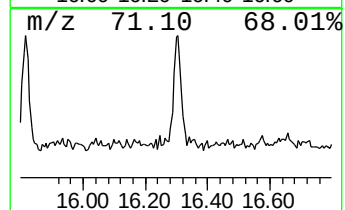
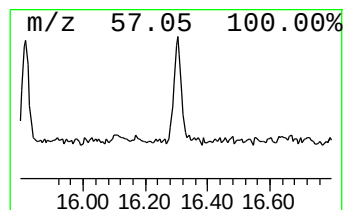
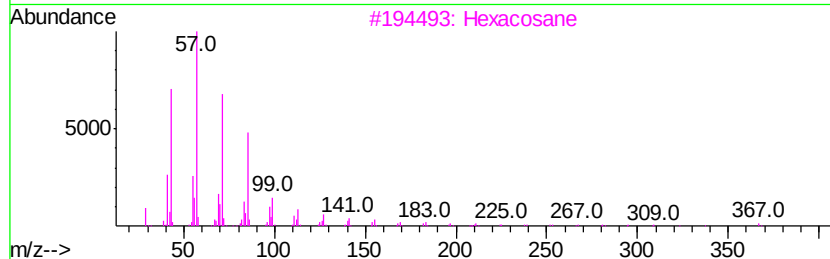
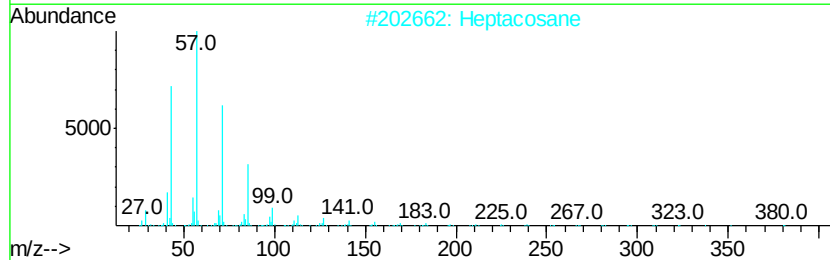
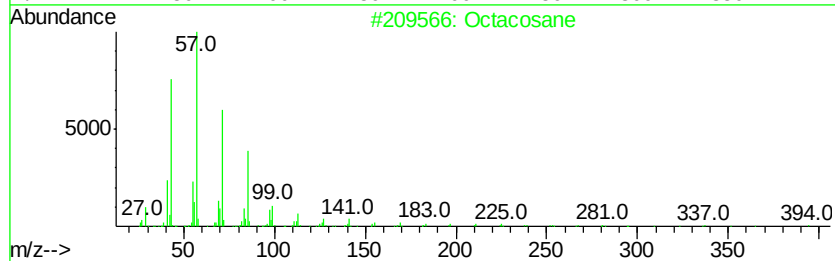
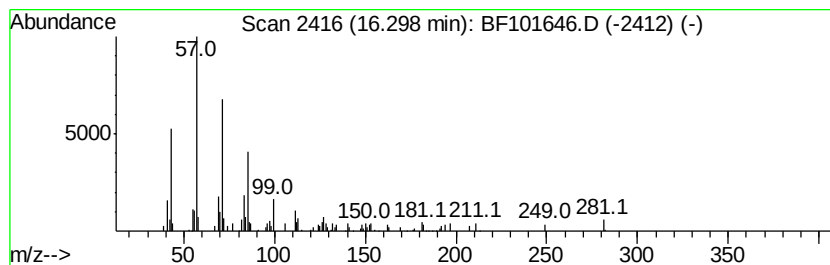
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	2.82 ng	89004	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptacosane	380	C27H56	000593-49-7	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		Hentriacontane	437	C31H64	000630-04-6	80
5		Heneicosane	296	C21H44	000629-94-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101646.D
Acq On : 22 Dec 2017 10:16
Operator : SJ/JU
Sample : I7008-12
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121817-TIFR-E-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.01	2.5	ng	103165	1	6.80	828729	20.0
unknown6.57	6.57	50.0	ng	2070300	1	6.80	828729	20.0
Hexadecanoic acid...	12.71	3.1	ng	131634	5	13.97	846554	20.0
Butyl myristate	13.41	2.5	ng	103958	5	13.97	846554	20.0
Heneicosane	15.82	2.5	ng	77151	6	15.44	630295	20.0
Octacosane	16.30	2.8	ng	89004	6	15.44	630295	20.0