

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092317\
 Data File : BF098771.D
 Acq On : 24 Sep 2017 7:23
 Operator : SJ/JU
 Sample : I5297-02
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091517-SIDI-E-D-S

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-BF092317.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	2.240	21	26	33	rVB	273785	351419	10.95%	1.630%
2	5.146	516	520	528	rVB	215357	212746	6.63%	0.987%
3	5.540	582	587	590	rBV	1373392	1263909	39.38%	5.864%
4	6.534	752	756	759	rBV	1038545	790571	24.63%	3.668%
5	6.563	759	761	765	rVB	42753	37465	1.17%	0.174%
6	6.687	778	782	786	rBV	2402845	2115014	65.91%	9.812%
7	6.922	818	822	828	rBV	993903	808766	25.20%	3.752%
8	7.081	844	849	852	rBV	3212237	2817166	87.78%	13.070%
9	7.487	912	918	921	rBV	2063913	2089918	65.12%	9.696%
10	8.204	1036	1040	1043	rVB	1081068	868387	27.06%	4.029%
11	9.281	1217	1223	1226	rBV	3507116	3209178	100.00%	14.888%
12	9.957	1334	1338	1342	rBV2	837009	714645	22.27%	3.315%
13	10.745	1468	1472	1475	rBV	1239770	1028751	32.06%	4.773%
14	11.445	1587	1591	1594	rBV	853833	660607	20.58%	3.065%
15	12.839	1825	1828	1832	rBV	65180	53966	1.68%	0.250%
16	13.033	1856	1861	1864	rBV	2732242	2676121	83.39%	12.415%
17	13.545	1945	1948	1951	rBV	56910	43739	1.36%	0.203%
18	14.086	2036	2040	2043	rBV	775829	738855	23.02%	3.428%
19	15.574	2288	2293	2304	rVB	457592	615037	19.16%	2.853%
20	16.045	2369	2373	2378	rVB	55143	80040	2.49%	0.371%
21	16.568	2457	2462	2467	rVB	67043	107685	3.36%	0.500%
22	17.180	2561	2566	2576	rVB3	48367	104686	3.26%	0.486%
23	17.909	2684	2690	2699	rVB3	40571	94445	2.94%	0.438%
24	18.768	2830	2836	2845	rVB6	24315	71669	2.23%	0.332%

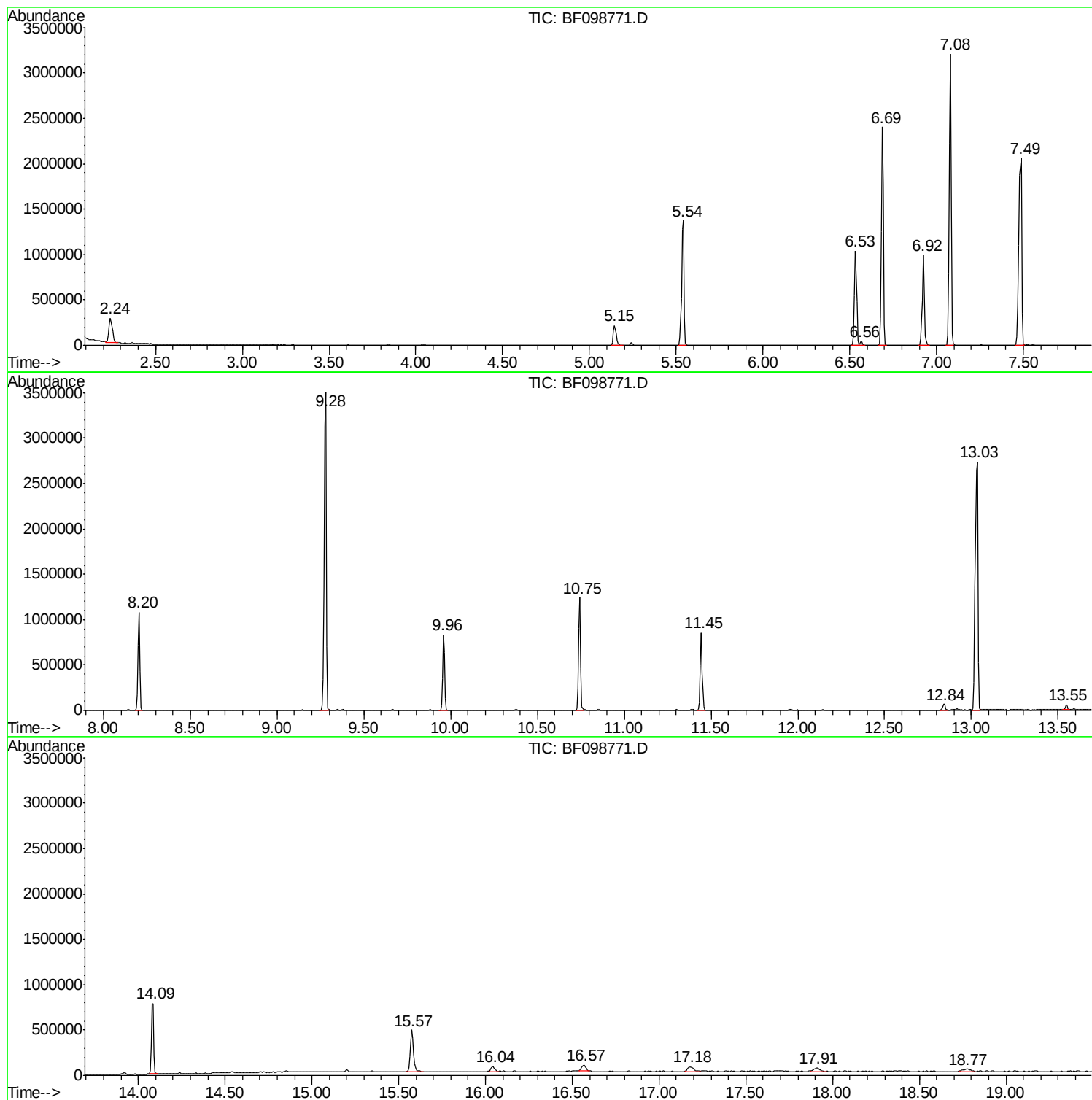
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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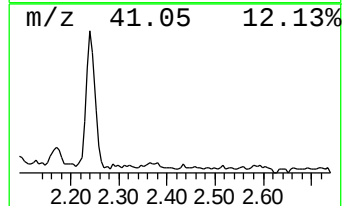
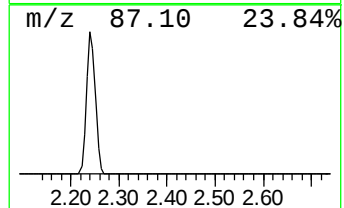
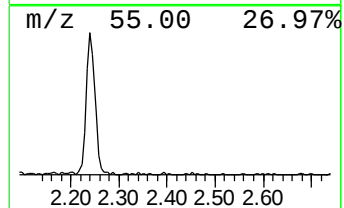
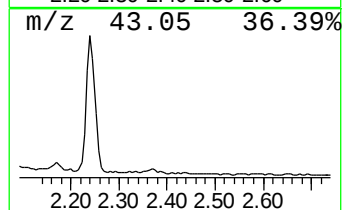
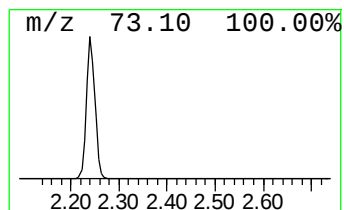
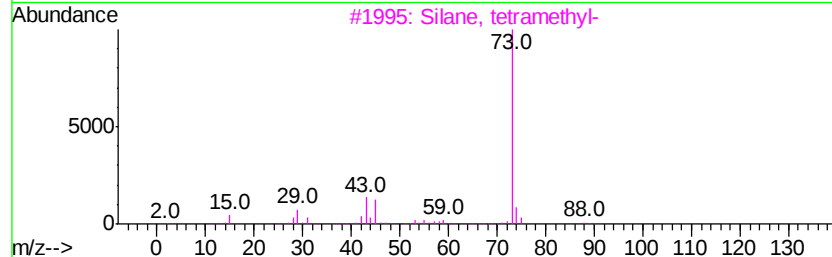
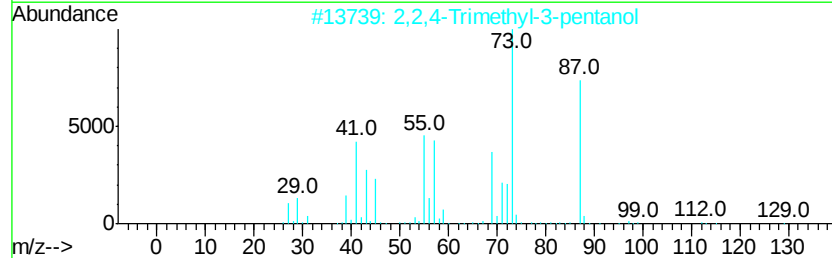
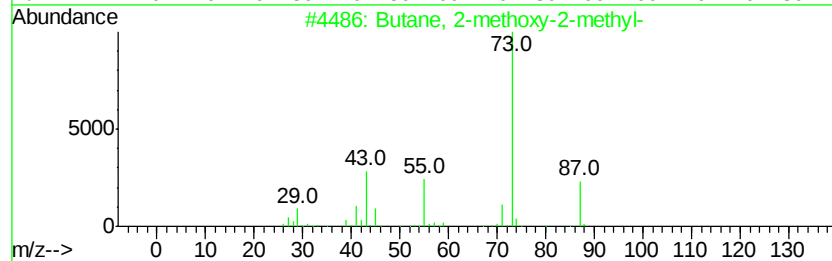
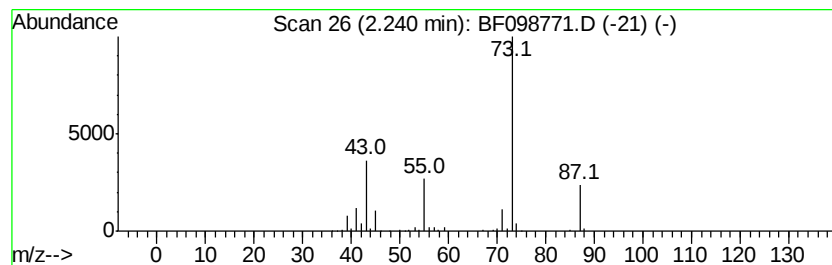
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	8.69 ng	351419	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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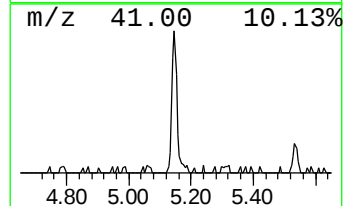
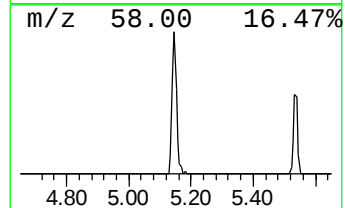
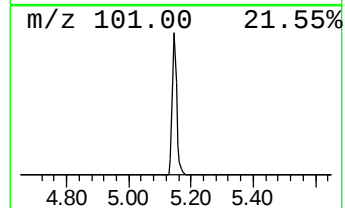
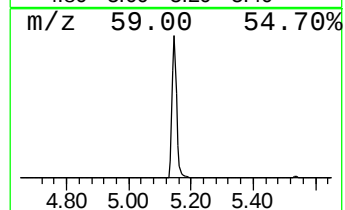
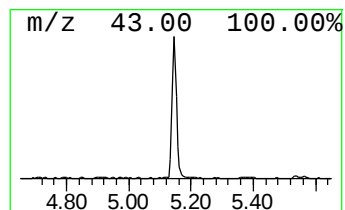
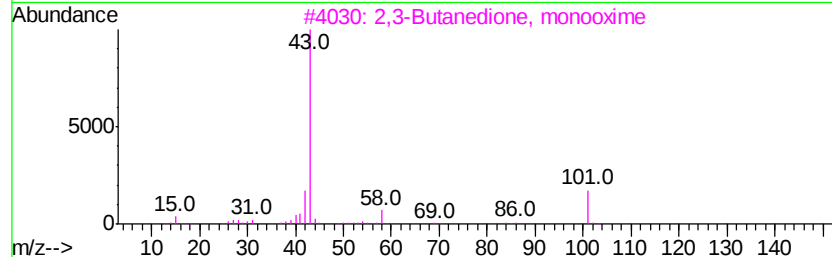
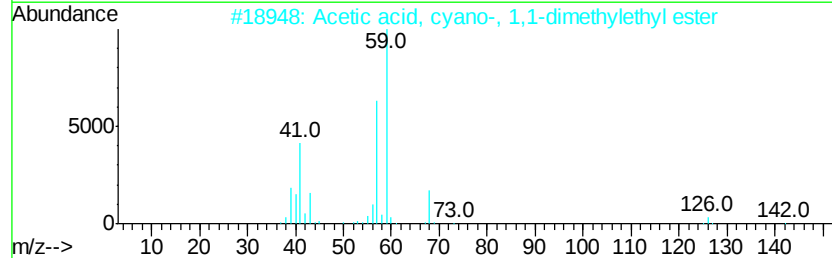
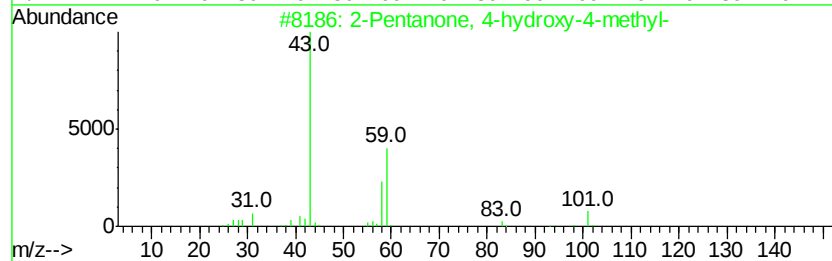
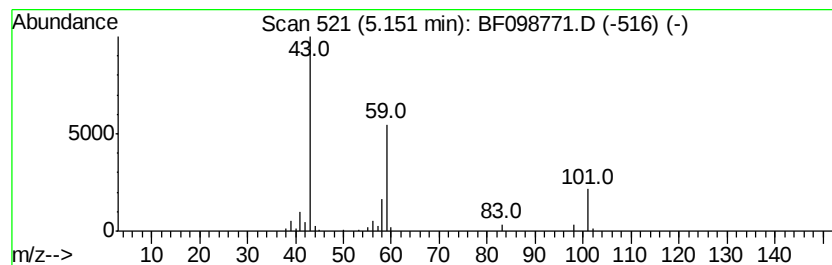
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.26 ng	212746	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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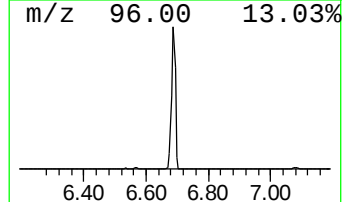
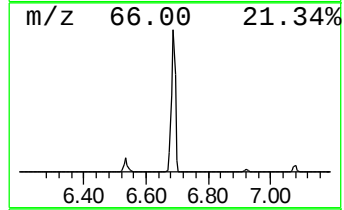
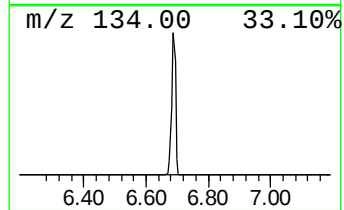
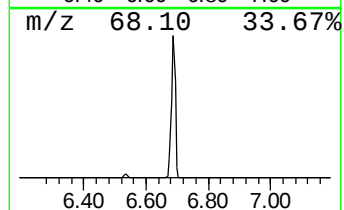
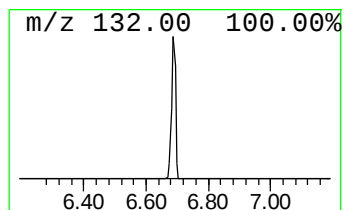
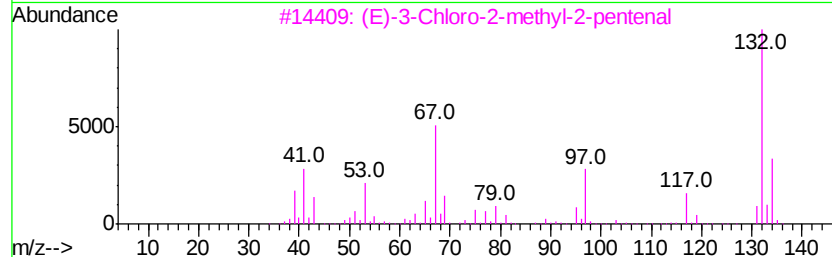
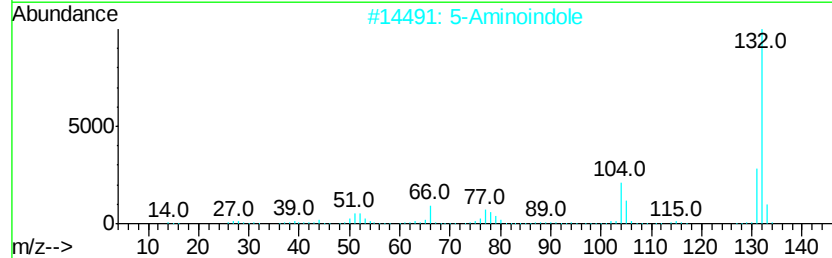
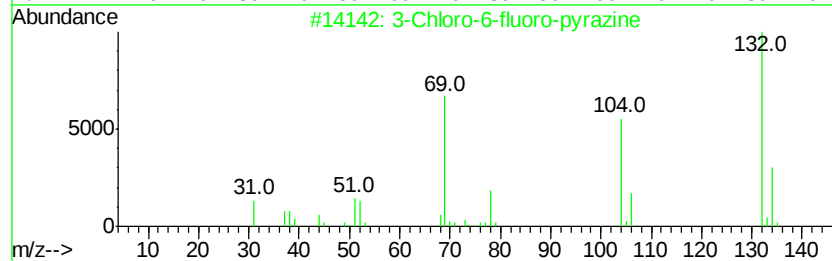
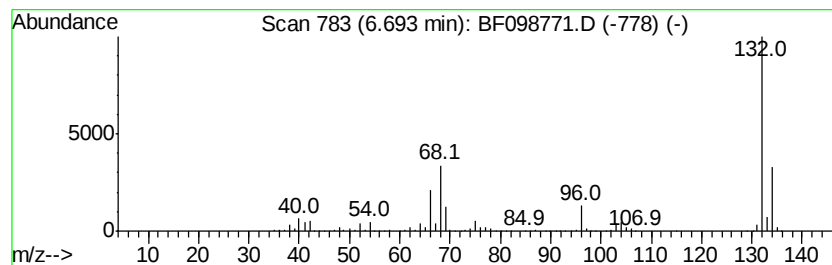
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Peak Number 3 unknown6.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	52.30 ng	2115010	1,4-Dichlorobenzene-d4	6.92

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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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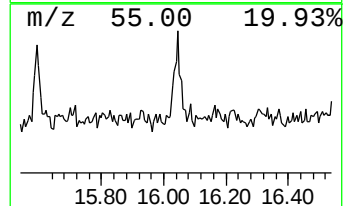
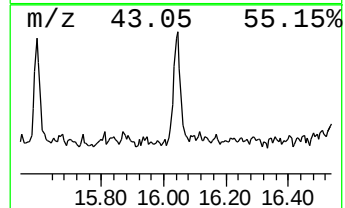
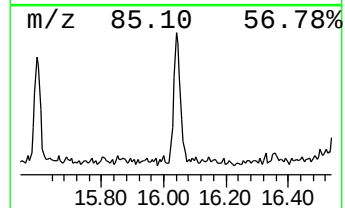
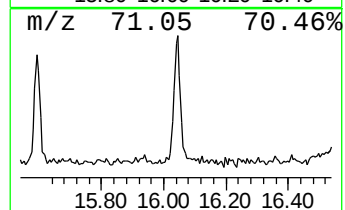
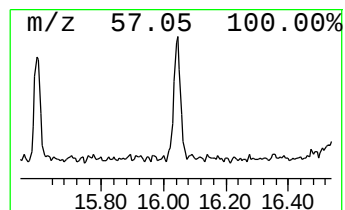
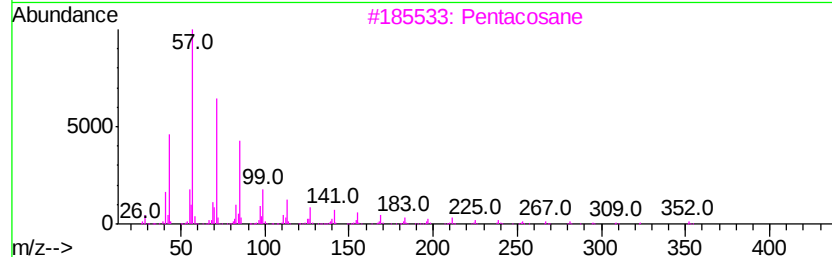
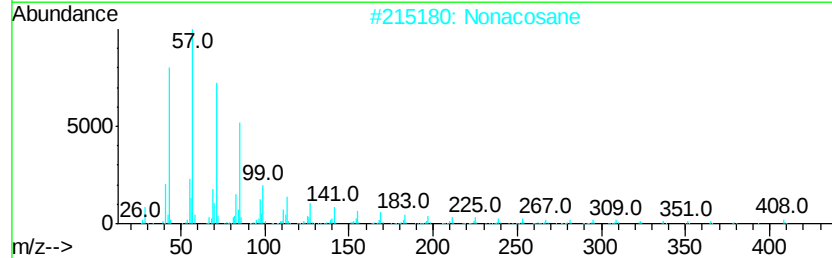
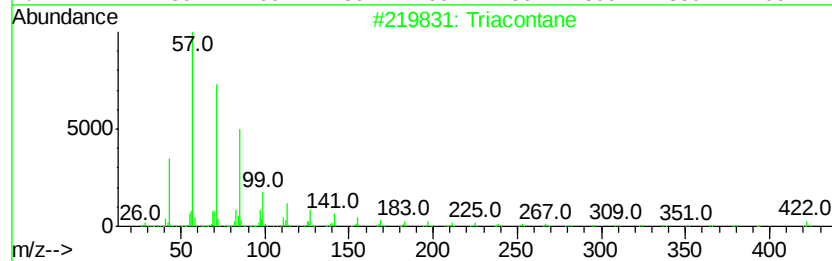
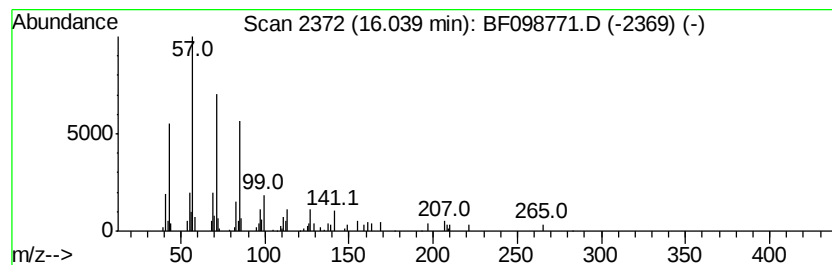
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Peak Number 5 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.60 ng	80040	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Nonacosane	408	C29H60	000630-03-5	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heptacosane	380	C27H56	000593-49-7	87



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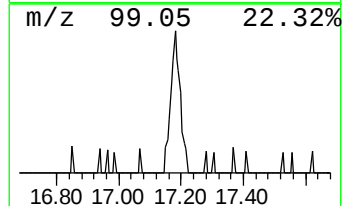
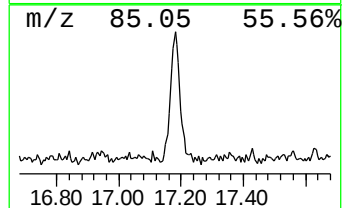
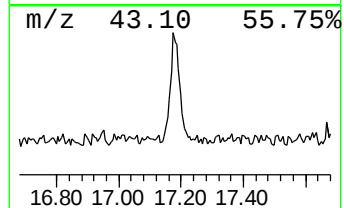
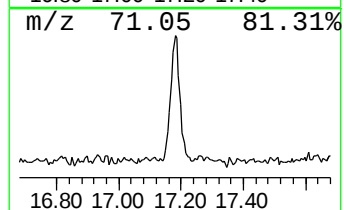
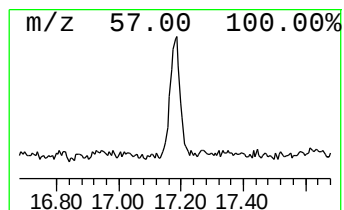
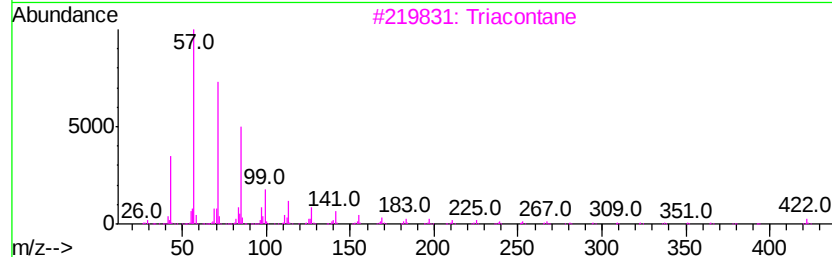
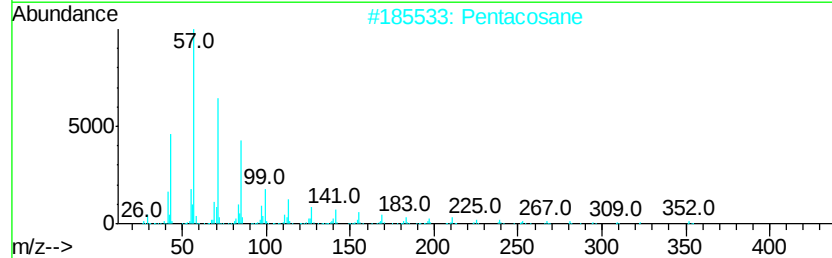
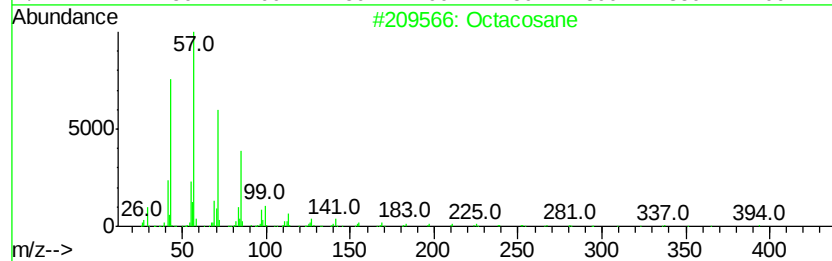
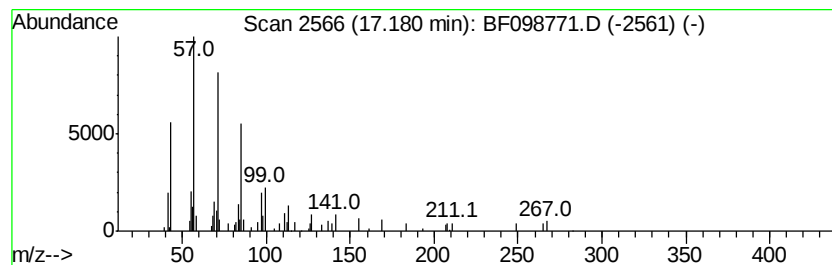
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.18	3.40 ng	104686	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Pentacosane	352	C25H52	000629-99-2	87
3		triacontane	422	C30H62	000638-68-6	83
4		Heneicosane	296	C21H44	000629-94-7	81
5		Hexacosane	366	C26H54	000630-01-3	81



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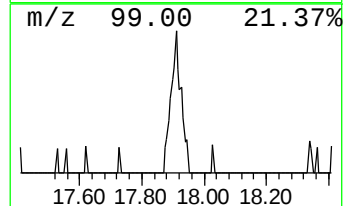
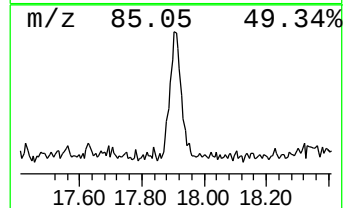
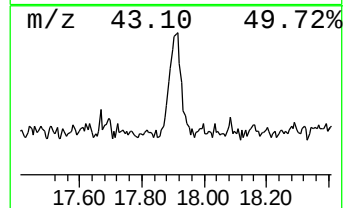
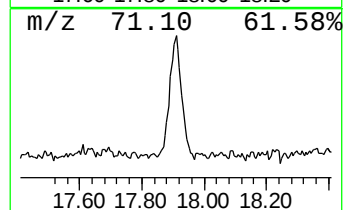
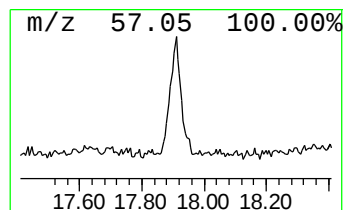
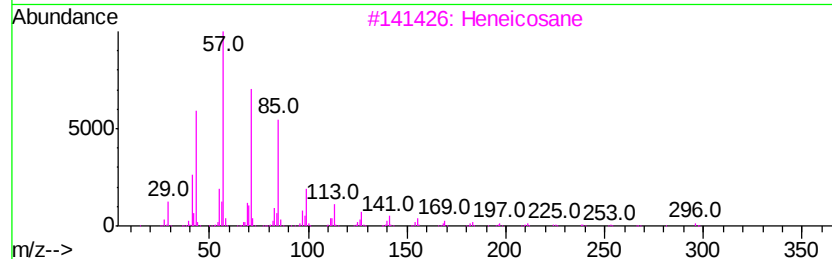
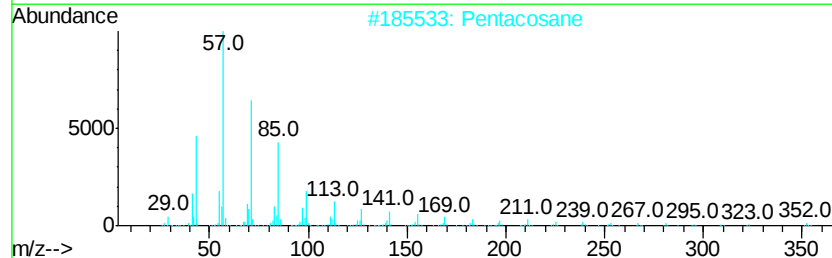
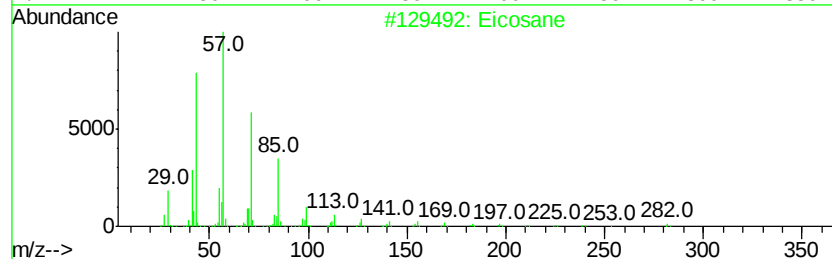
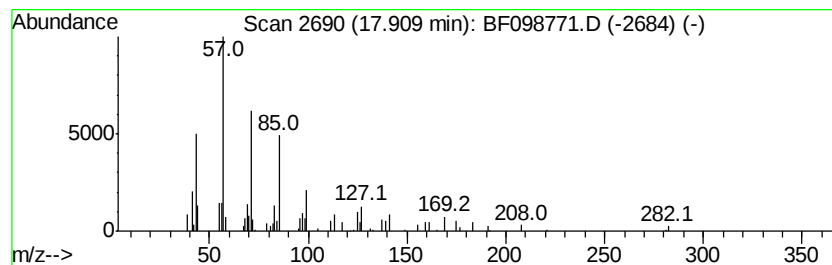
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	3.07 ng	94445	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	81
2	Pentacosane		352	C25H52	000629-99-2	74
3	Heneicosane		296	C21H44	000629-94-7	72
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	72
5	Hexacosane		366	C26H54	000630-01-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092317\
Data File : BF098771.D
Acq On : 24 Sep 2017 7:23
Operator : SJ/JU
Sample : I5297-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091517-SIDI-E-D-S

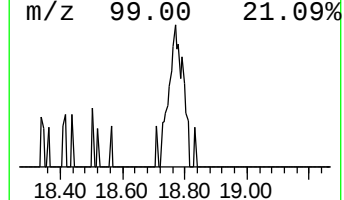
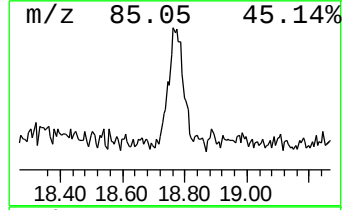
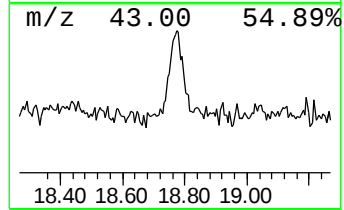
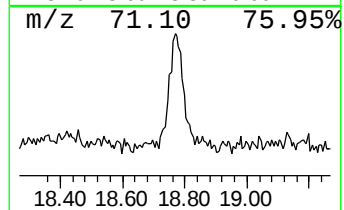
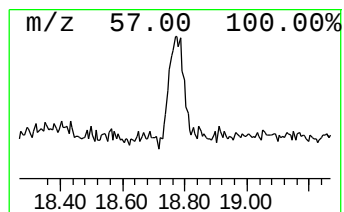
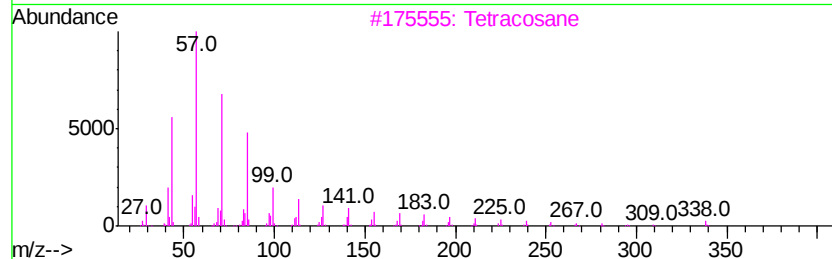
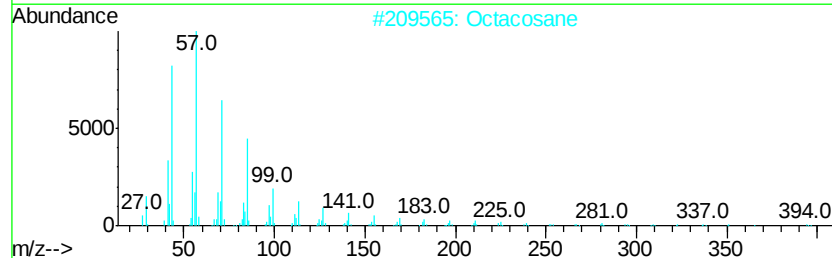
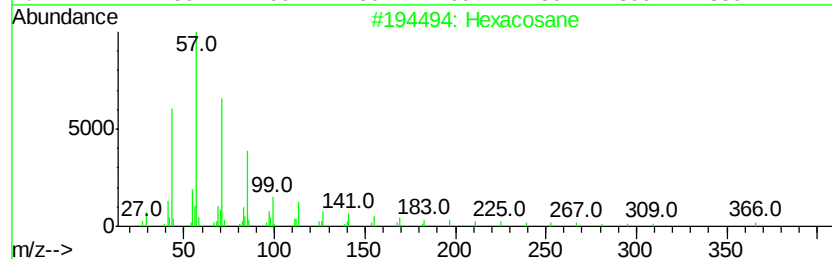
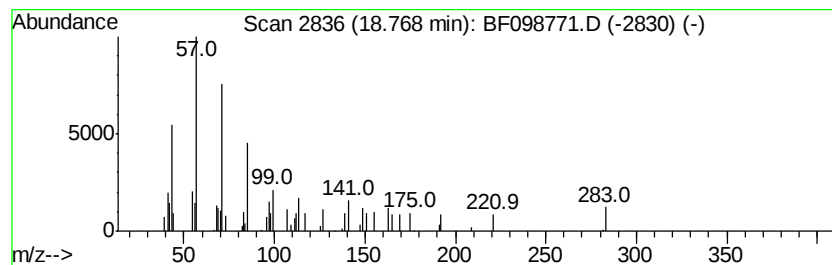
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	2.33 ng	71669	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	62
2	Octacosane		394	C28H58	000630-02-4	58
3	Tetracosane		338	C24H50	000646-31-1	58
4	Pentacosane		352	C25H52	000629-99-2	58
5	Tetracontane		563	C40H82	004181-95-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092317\
Data File : BF098771.D
Acq On : 24 Sep 2017 7:23
Operator : SJ/JU
Sample : I5297-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091517-SIDI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.24	8.7	ng	351419	1	6.92	808766	20.0
2-Pentanone, 4-hy...	5.15	5.3	ng	212746	1	6.92	808766	20.0
unknown6.69	6.69	52.3	ng	2115010	1	6.92	808766	20.0
Triacontane	16.04	2.6	ng	80040	6	15.57	615037	20.0
Octacosane	17.18	3.4	ng	104686	6	15.57	615037	20.0
Eicosane	17.91	3.1	ng	94445	6	15.57	615037	20.0
Hexacosane	18.77	2.3	ng	71669	6	15.57	615037	20.0