

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052317\
 Data File : BF095366.D
 Acq On : 23 May 2017 23:42
 Operator : SJ/MA
 Sample : I3249-12
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-17COMP

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-BF050217.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	5.125	538	542	556	rBV	115787	265784	8.14%	1.150%
2	5.719	639	643	684	rBV	1079728	2504911	76.71%	10.842%
3	7.295	907	911	928	rBV	1325528	2317605	70.98%	10.031%
4	7.419	928	932	946	rVB	1729828	2768176	84.77%	11.982%
5	7.754	985	989	1001	rBV	454714	536977	16.44%	2.324%
6	7.989	1024	1029	1049	rVB	1659605	2052732	62.86%	8.885%
7	8.654	1138	1142	1169	rBV	844636	1489372	45.61%	6.446%
8	9.777	1328	1333	1350	rBV	390723	738359	22.61%	3.196%
9	11.542	1628	1633	1661	rBV	2236354	3265366	100.00%	14.134%
10	12.248	1749	1753	1771	rBV	208989	358006	10.96%	1.550%
11	12.607	1809	1814	1826	rBV2	519389	841897	25.78%	3.644%
12	13.436	1951	1955	1961	rVB	45348	49532	1.52%	0.214%
13	13.901	2029	2034	2055	rBV	880753	1601901	49.06%	6.934%
14	14.207	2083	2086	2095	rBV	38156	55580	1.70%	0.241%
15	15.012	2219	2223	2246	rVB	393368	692414	21.20%	2.997%
16	15.965	2381	2385	2395	rBV3	62626	110058	3.37%	0.476%
17	17.330	2612	2617	2638	rBV	1764587	2204817	67.52%	9.543%
18	18.089	2742	2746	2747	rVV	32386	33645	1.03%	0.146%
19	18.106	2747	2749	2753	rVB	36353	35754	1.09%	0.155%
20	18.577	2825	2829	2844	rBV5	31179	97218	2.98%	0.421%
21	18.689	2844	2848	2861	rBV	255967	428194	13.11%	1.853%
22	20.083	3081	3085	3090	rBV2	28622	36689	1.12%	0.159%
23	20.365	3129	3133	3141	rBV2	245999	440298	13.48%	1.906%
24	20.430	3141	3144	3150	rVB2	38245	54026	1.65%	0.234%
25	20.806	3205	3208	3212	rBV3	25861	33148	1.02%	0.143%
26	21.241	3278	3282	3287	rVB2	26262	41765	1.28%	0.181%
27	21.736	3361	3366	3375	rBV8	21419	49498	1.52%	0.214%

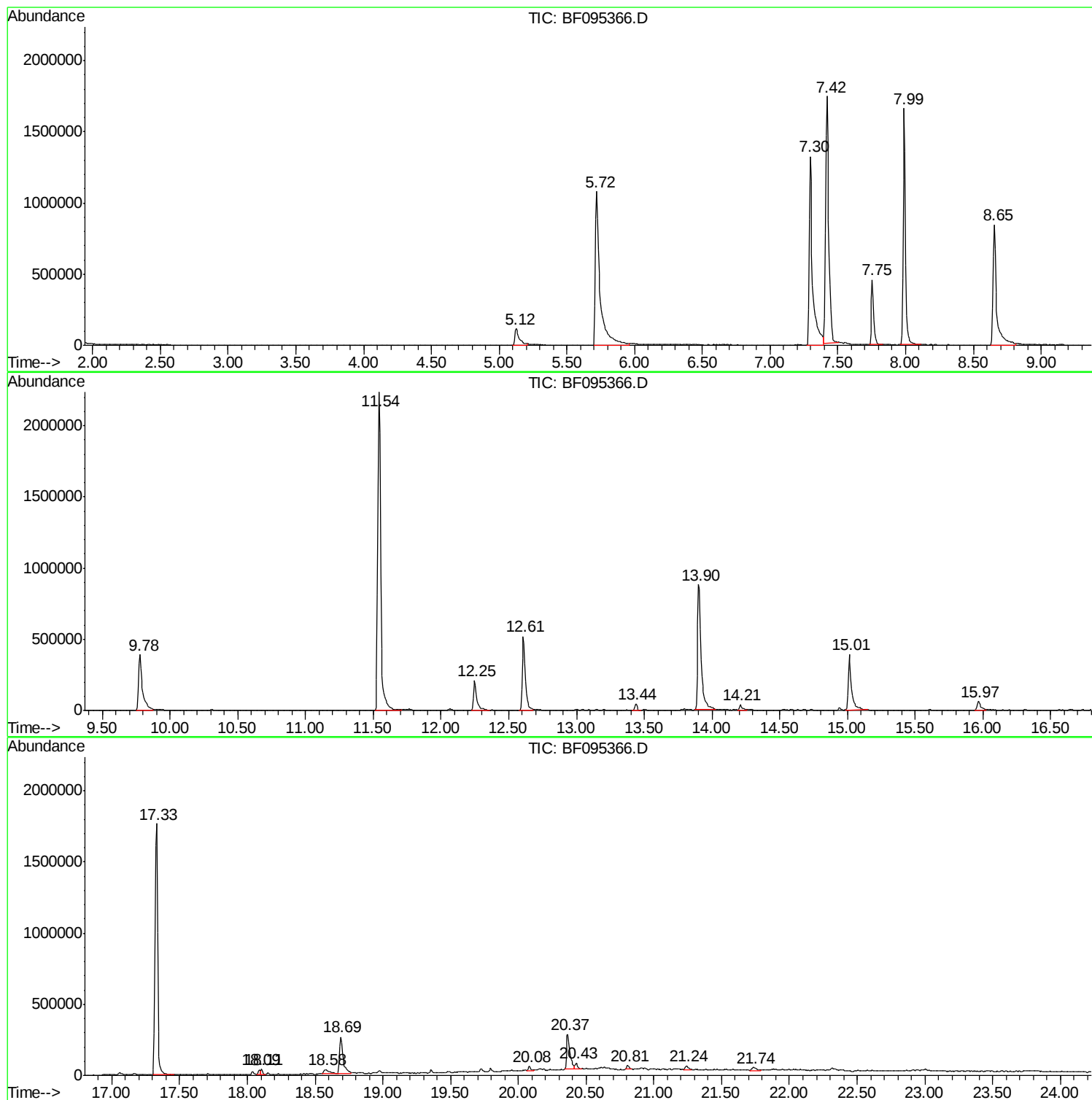
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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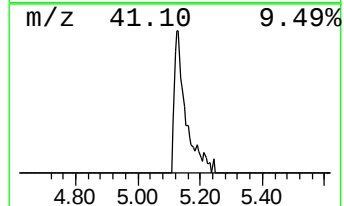
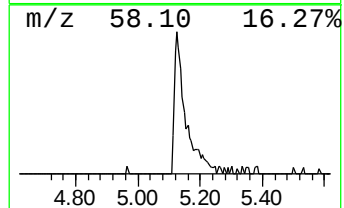
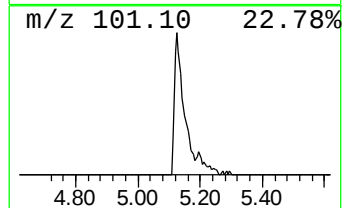
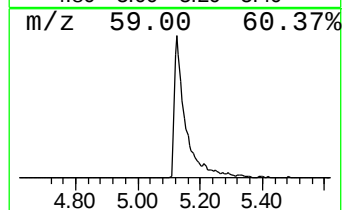
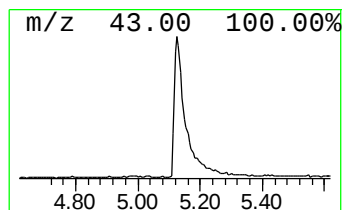
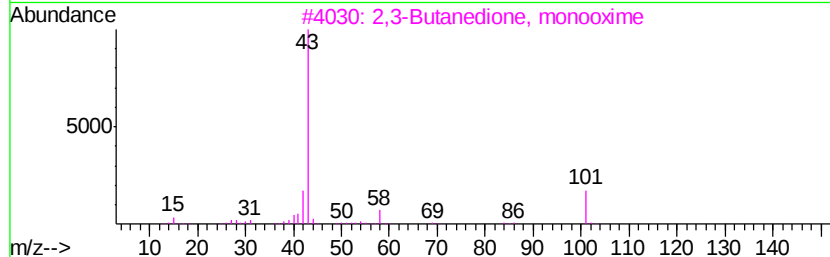
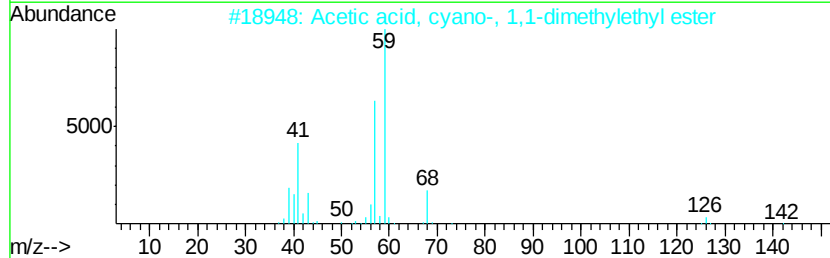
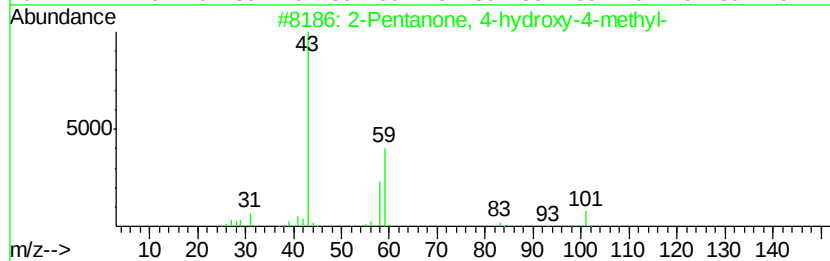
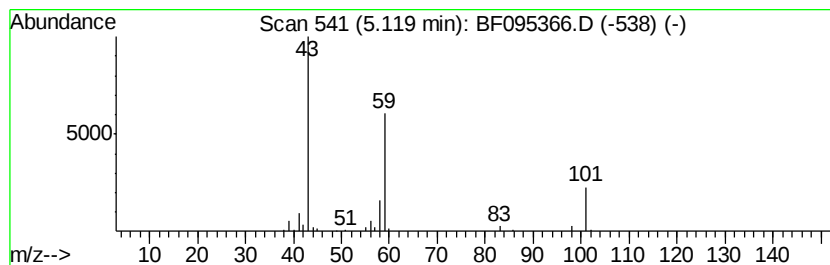
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	9.90 ng	265784	1,4-Dichlorobenzene-d4	7.75

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-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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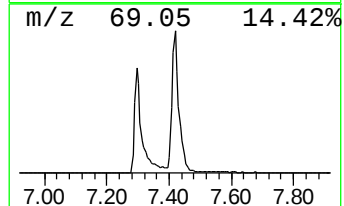
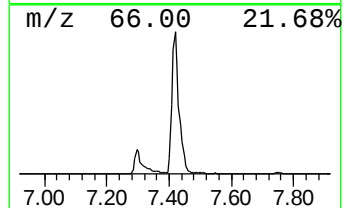
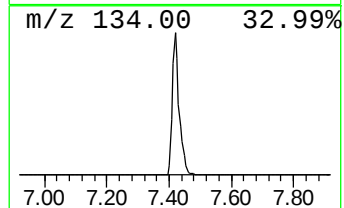
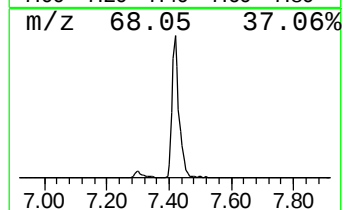
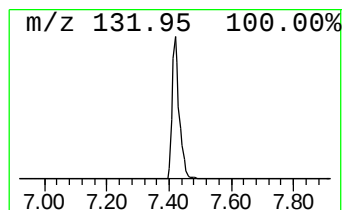
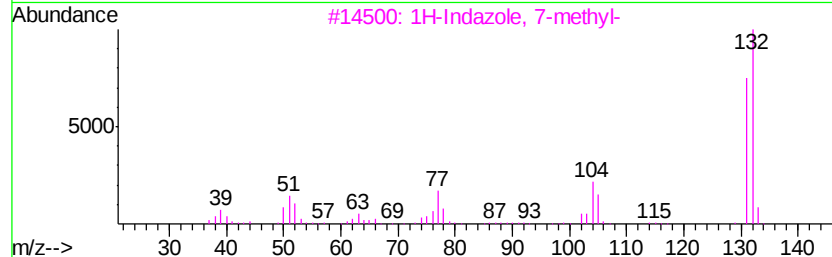
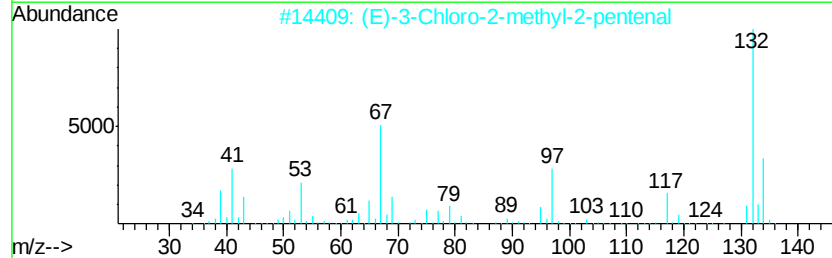
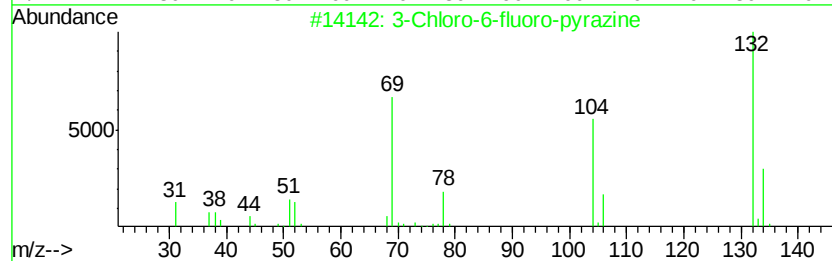
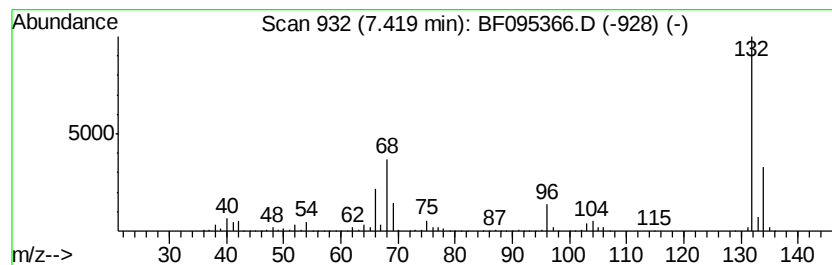
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	103.10 ng	2768180	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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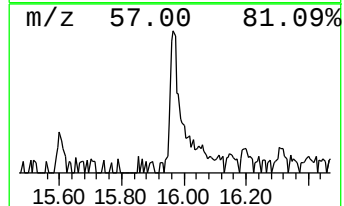
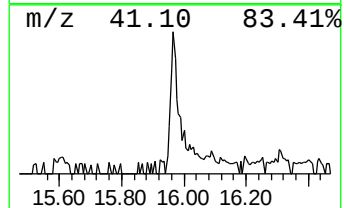
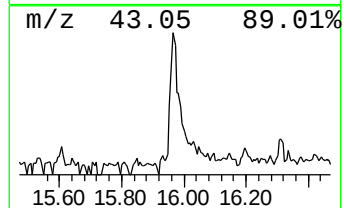
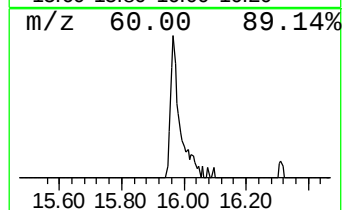
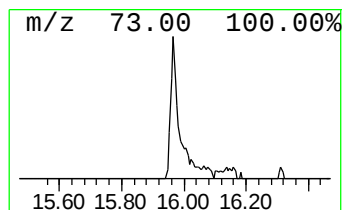
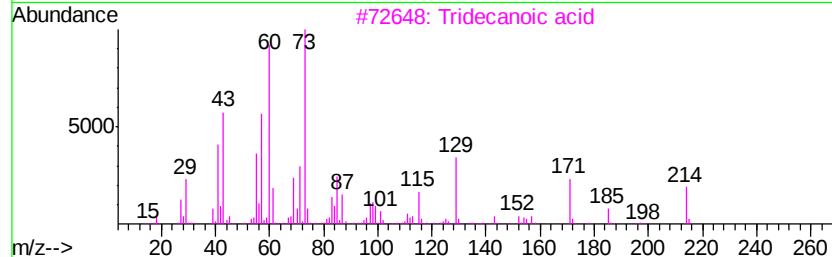
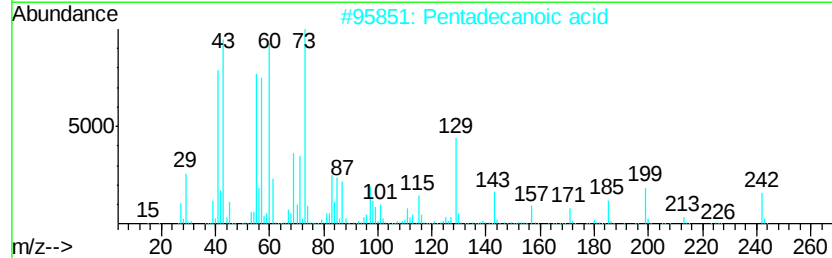
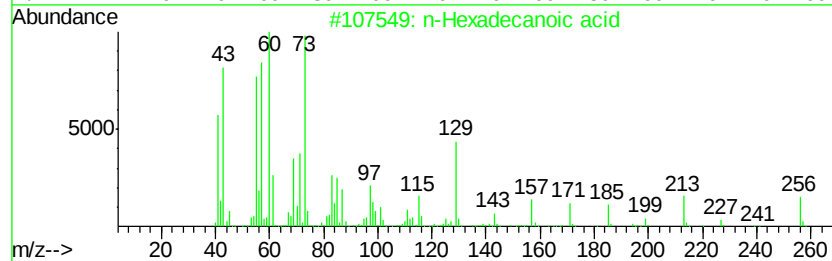
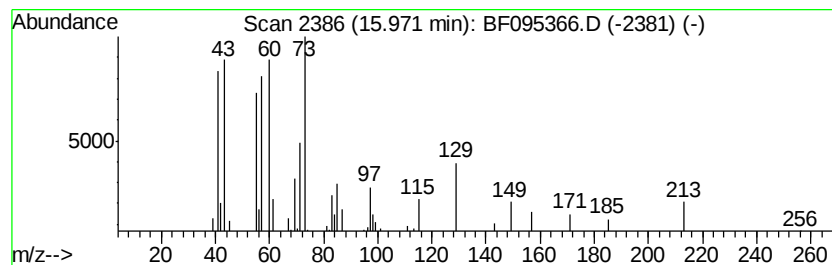
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.18 ng	110058	Phenanthrene-d10	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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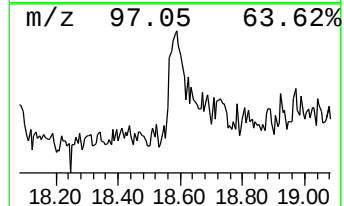
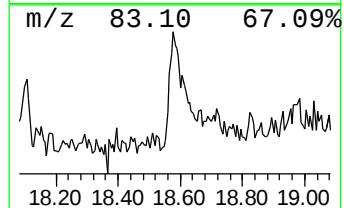
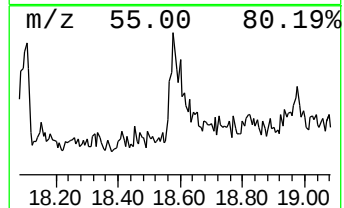
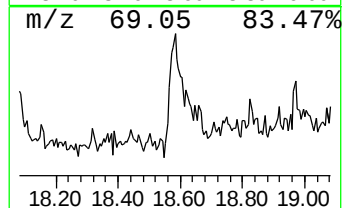
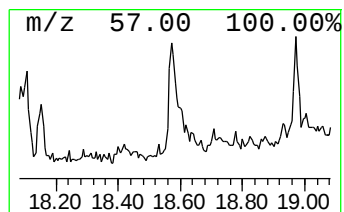
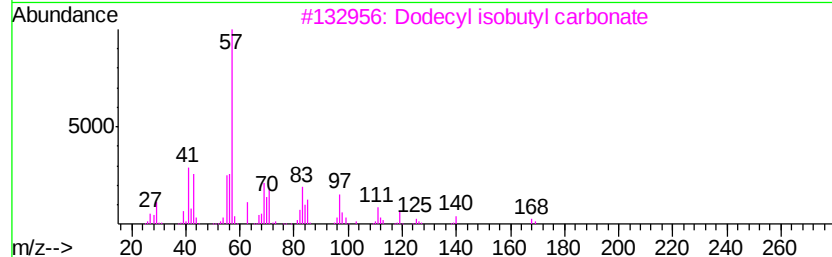
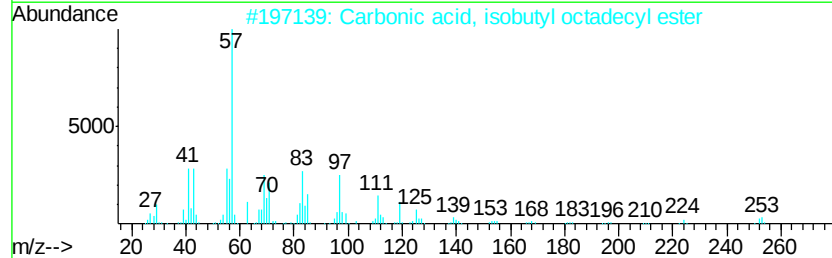
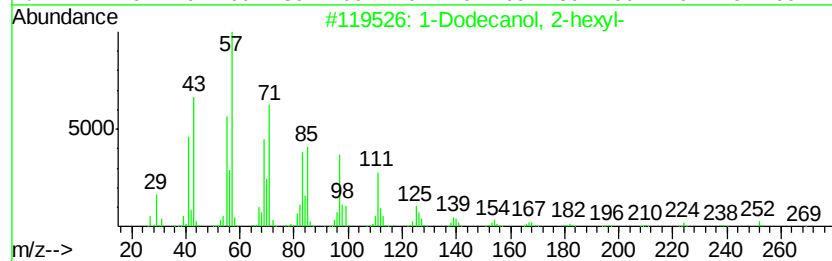
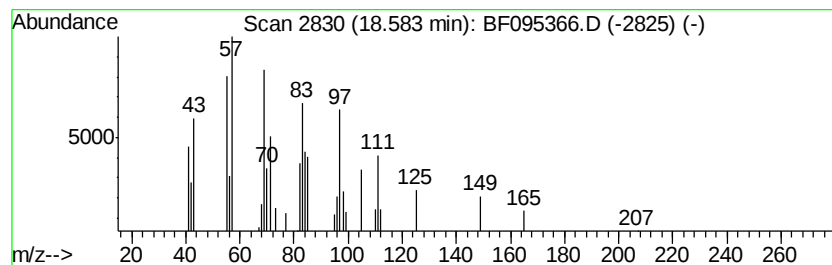
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Dodecanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.58	4.54 ng	97218	Chrysene-d12	18.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	59
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	53
3	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	53
4	Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	52
5	17-Pentatriacontene	491	C35H70	006971-40-0	47



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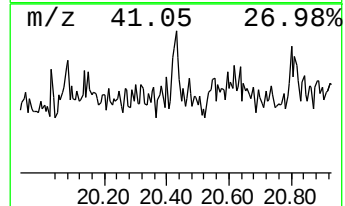
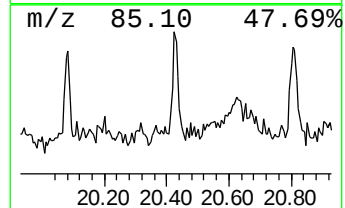
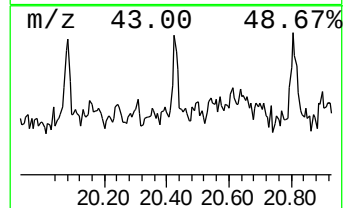
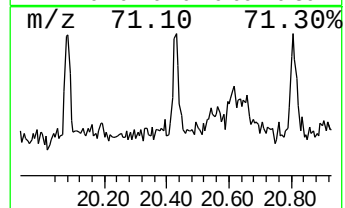
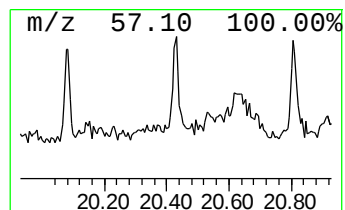
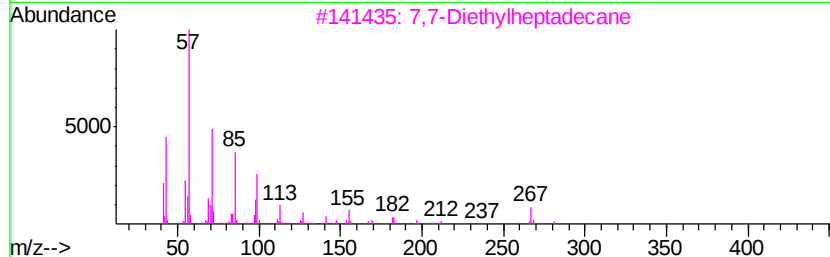
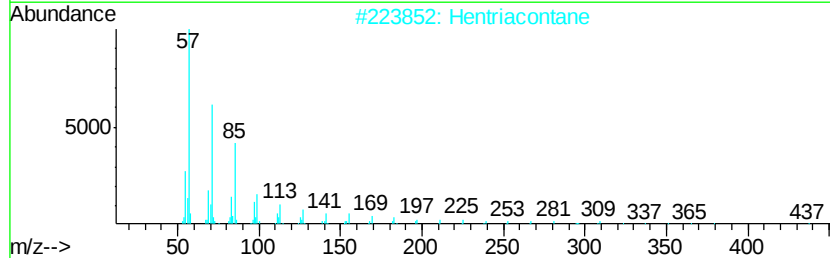
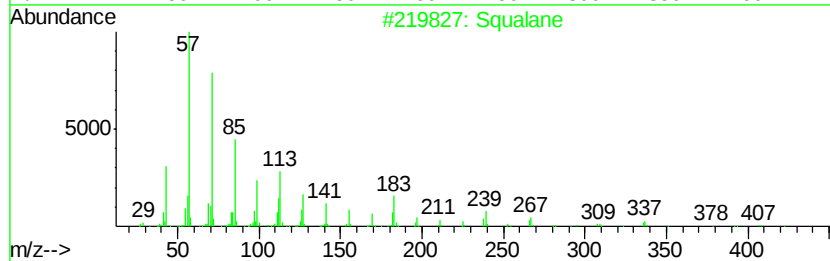
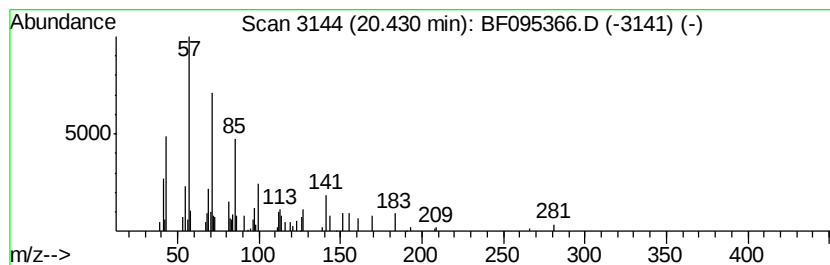
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	2.45 ng	54026	Perylene-d12	20.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalane	422 C30H62	000111-01-3	72
2	Hentriacontane	437 C31H64	000630-04-6	64
3	7,7-Diethylheptadecane	296 C21H44	1000360-41-5	64
4	Hexacosane	366 C26H54	000630-01-3	59
5	Sulfurous acid, butyl tridecyl e...	320 C17H36O3S	1000309-18-0	59



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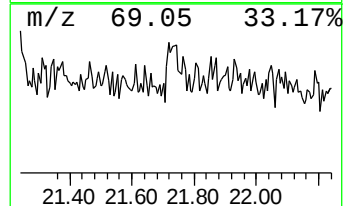
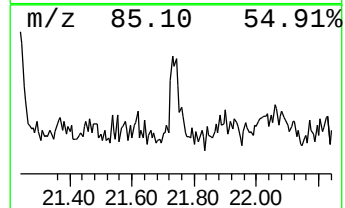
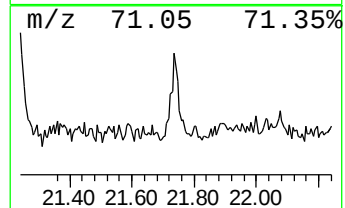
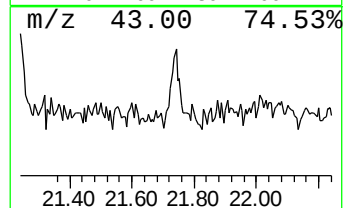
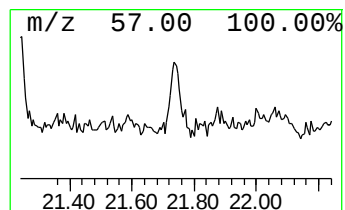
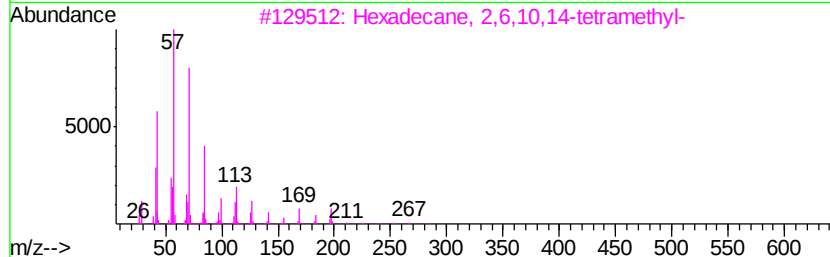
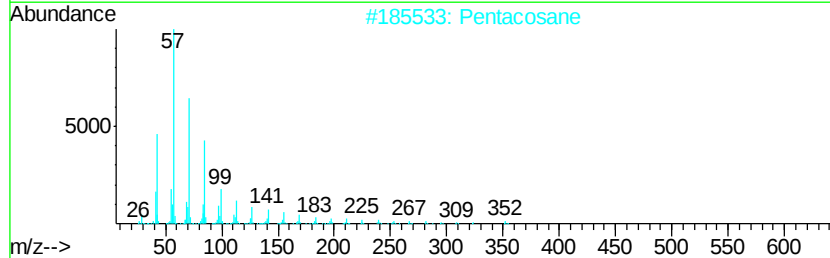
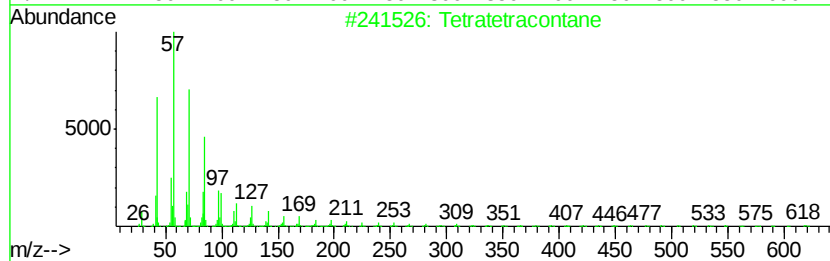
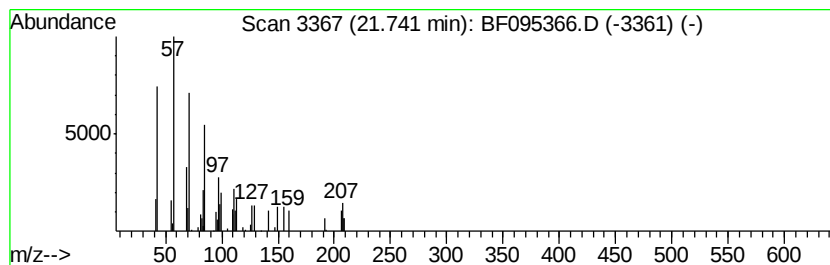
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	2.25 ng	49498	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	64
2		Pentacosane	352	C25H52	000629-99-2	59
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
4		Hexacosane	366	C26H54	000630-01-3	53
5		Octadecane	254	C18H38	000593-45-3	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052317\
Data File : BF095366.D
Acq On : 23 May 2017 23:42
Operator : SJ/MA
Sample : I3249-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.12	9.9	ng	265784	1	7.75	536977	20.0
unknown7.42	7.42	103.1	ng	2768180	1	7.75	536977	20.0
n-Hexadecanoic acid	15.97	3.2	ng	110058	4	15.01	692414	20.0
1-Dodecanol, 2-he...	18.58	4.5	ng	97218	5	18.69	428194	20.0
Squalane	20.43	2.5	ng	54026	6	20.36	440298	20.0
Tetratetracontane	21.74	2.3	ng	49498	6	20.36	440298	20.0