

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
 Data File : BF095687.D
 Acq On : 5 Jun 2017 22:41
 Operator : SJ/MA
 Sample : I3438-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-8-9

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-BF060517.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	1.602	8	11	46	rVB	841175	1784691	52.96%	5.693%
2	4.637	522	527	552	rBV	94279	302545	8.98%	0.965%
3	5.301	635	640	671	rBV	1957992	3265773	96.92%	10.418%
4	6.960	916	922	933	rBV	1847369	3015245	89.48%	9.619%
5	7.060	933	939	953	rVB	2203129	3273046	97.13%	10.441%
6	7.395	992	996	1009	rBV	439168	580242	17.22%	1.851%
7	7.637	1031	1037	1055	rBV	1896558	2550078	75.68%	8.135%
8	8.313	1146	1152	1172	rBV	1257808	1984961	58.91%	6.332%
9	9.425	1337	1341	1354	rBV	657298	844666	25.07%	2.695%
10	11.213	1637	1645	1660	rVB	2479976	3369603	100.00%	10.750%
11	11.901	1756	1762	1769	rBV	630304	735938	21.84%	2.348%
12	12.248	1814	1821	1826	rBV2	764690	949800	28.19%	3.030%
13	12.295	1826	1829	1834	rVB	65463	76750	2.28%	0.245%
14	13.107	1961	1967	1972	rBV	73592	95364	2.83%	0.304%
15	13.466	2019	2028	2032	rBV2	24900	50959	1.51%	0.163%
16	13.548	2036	2042	2049	rVV	1352956	1918084	56.92%	6.119%
17	13.877	2094	2098	2108	rBV	96930	148621	4.41%	0.474%
18	14.607	2217	2222	2224	rBV	89261	108169	3.21%	0.345%
19	14.642	2224	2228	2241	rVB	688219	880405	26.13%	2.809%
20	15.289	2333	2338	2342	rBV	70406	83971	2.49%	0.268%
21	15.442	2360	2364	2369	rVB	33605	37868	1.12%	0.121%
22	15.660	2394	2401	2409	rBV	137788	193469	5.74%	0.617%
23	15.889	2436	2440	2447	rBV	49330	63012	1.87%	0.201%
24	16.412	2524	2529	2531	rBV	79553	88154	2.62%	0.281%
25	16.442	2531	2534	2537	rVB	93274	86062	2.55%	0.275%
26	16.759	2584	2588	2594	rBV2	37915	60736	1.80%	0.194%
27	17.018	2625	2632	2635	rBV	2109541	2710355	80.44%	8.646%
28	18.265	2840	2844	2854	rBV	105229	159570	4.74%	0.509%
29	18.354	2854	2859	2869	rVB	457860	551884	16.38%	1.761%
30	18.595	2893	2900	2903	rBV2	32870	41868	1.24%	0.134%
31	19.395	3031	3036	3046	rBV	645525	780984	23.18%	2.491%
32	20.018	3138	3142	3150	rBV	437401	553694	16.43%	1.766%

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ClientSampleId :
TP-8-9

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

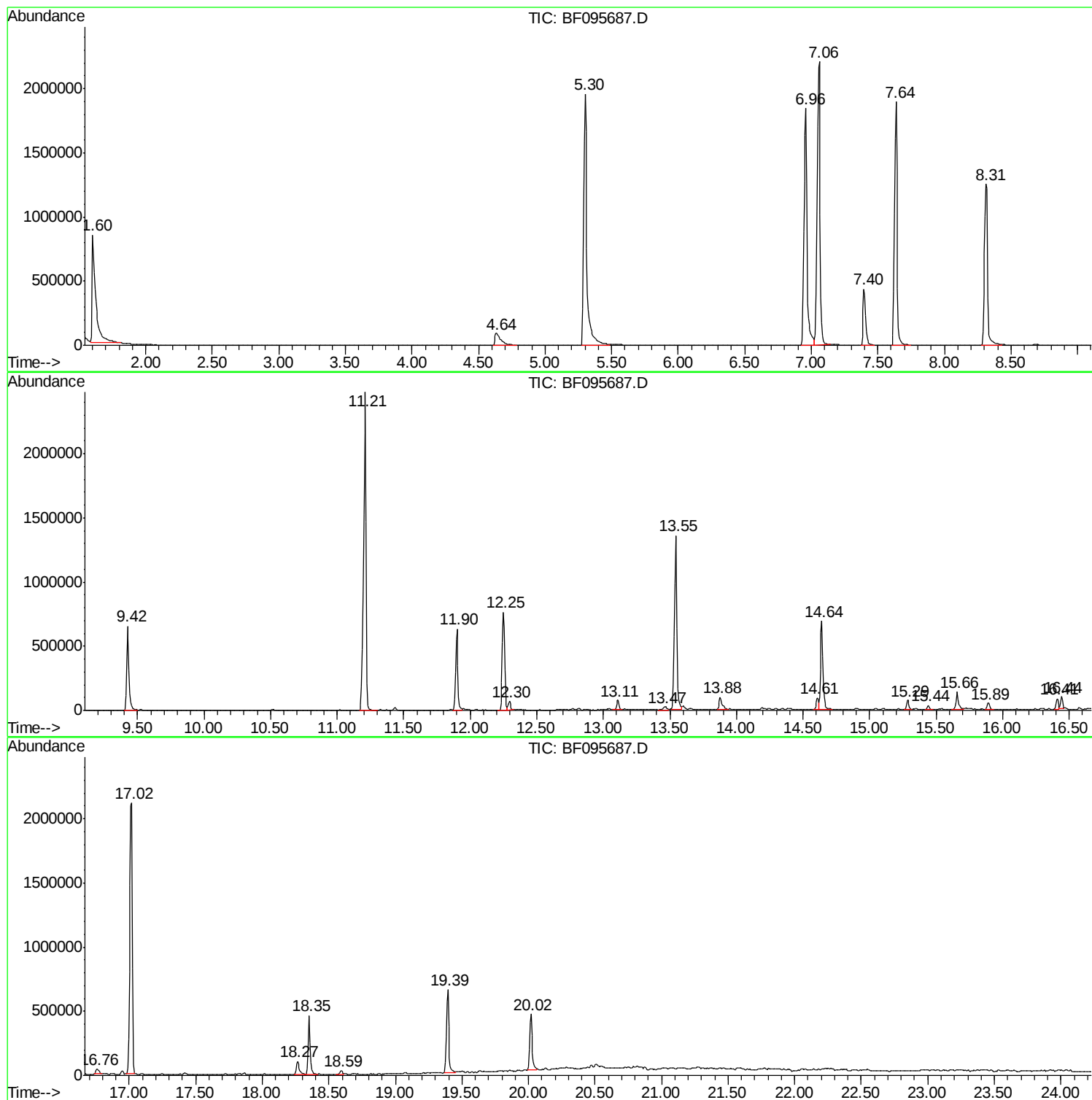
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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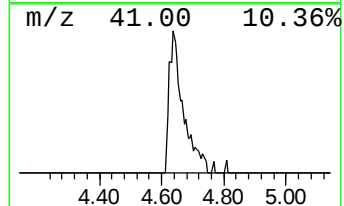
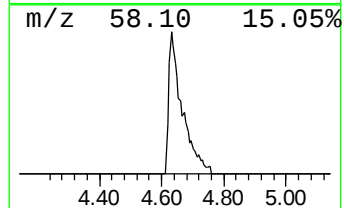
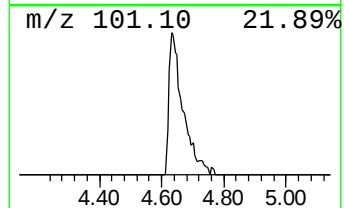
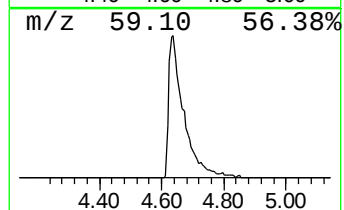
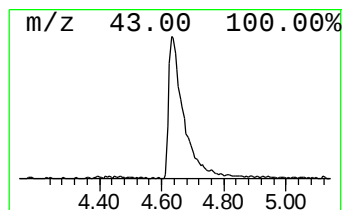
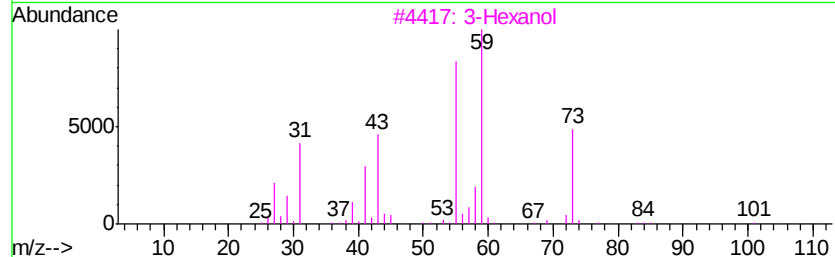
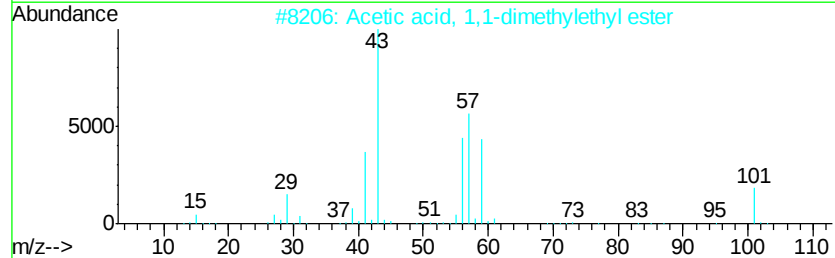
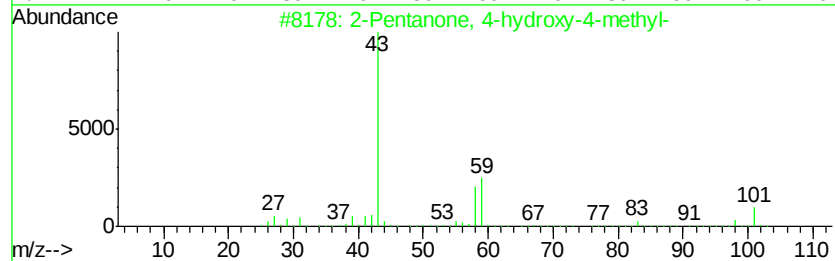
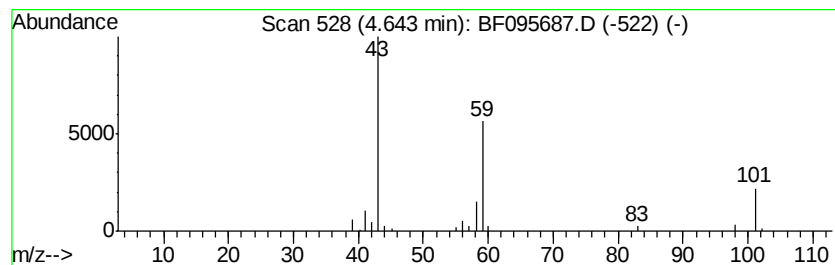
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	10.43 ng	302545	1,4-Dichlorobenzene-d4	7.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Hexanol	102	C6H14O	000623-37-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25



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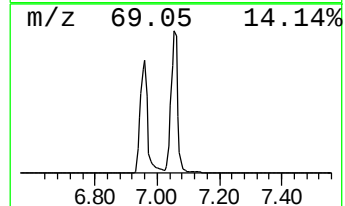
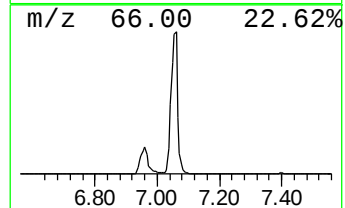
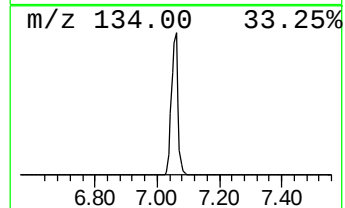
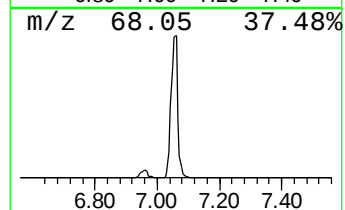
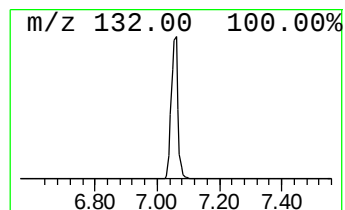
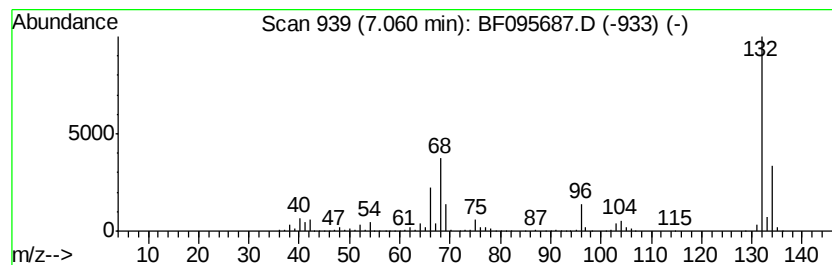
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	112.82 ng	3273050	1,4-Dichlorobenzene-d4	7.40

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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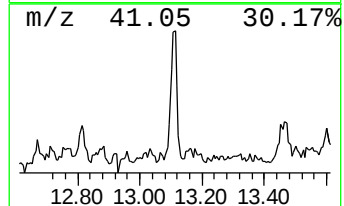
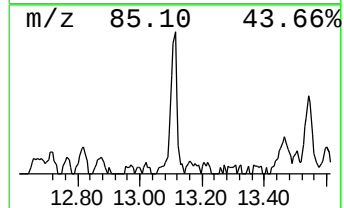
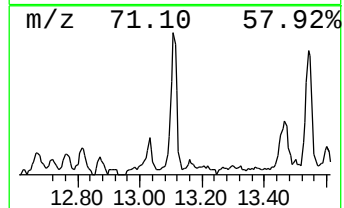
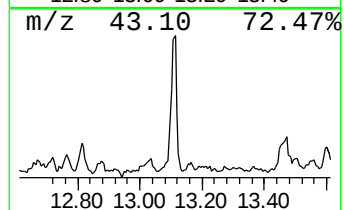
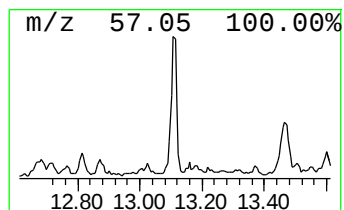
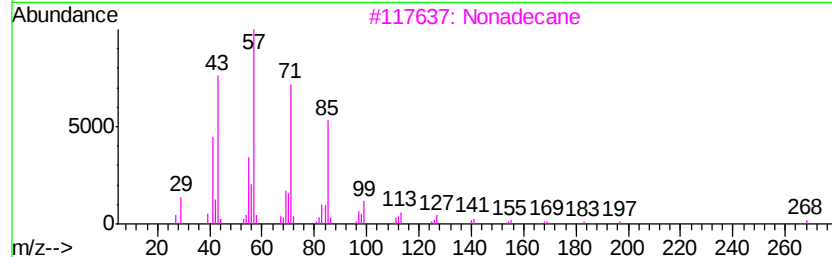
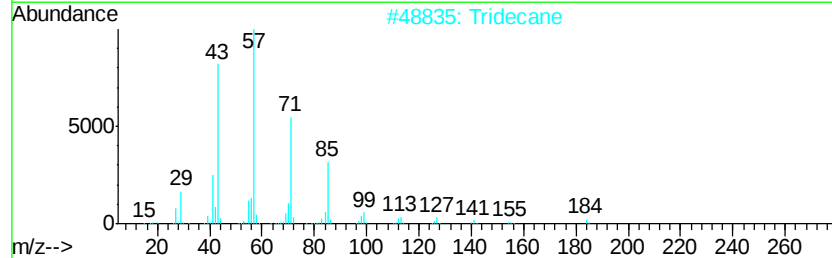
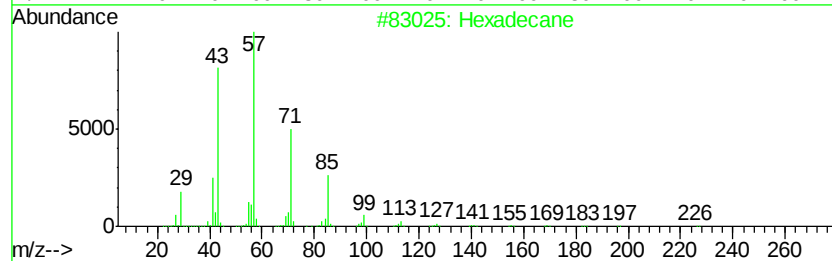
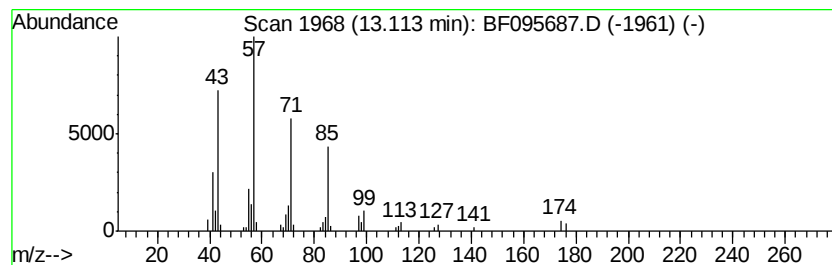
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	2.01 ng	95364	Acenaphthene-d10	12.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	86
2	Tridecane		184	C13H28	000629-50-5	80
3	Nonadecane		268	C19H40	000629-92-5	80
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	80
5	Tetradecane		198	C14H30	000629-59-4	72



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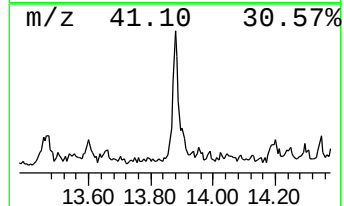
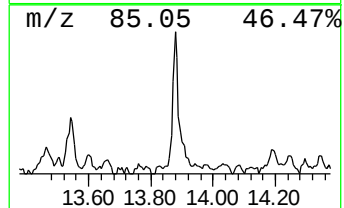
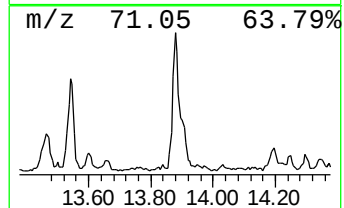
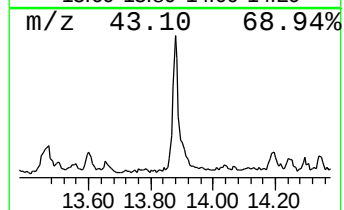
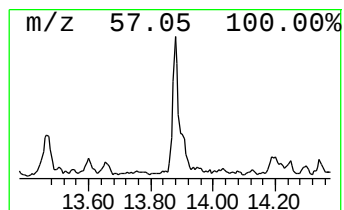
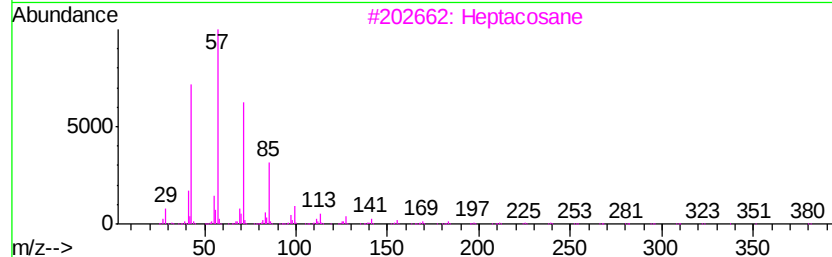
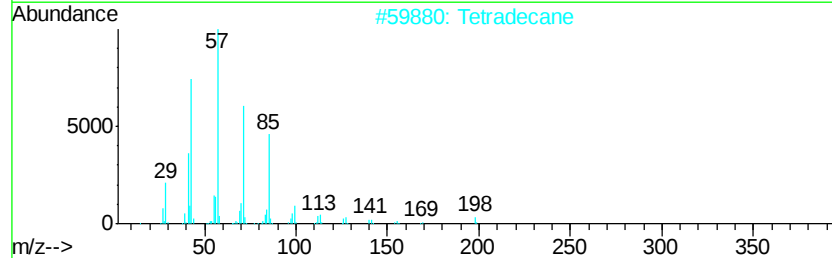
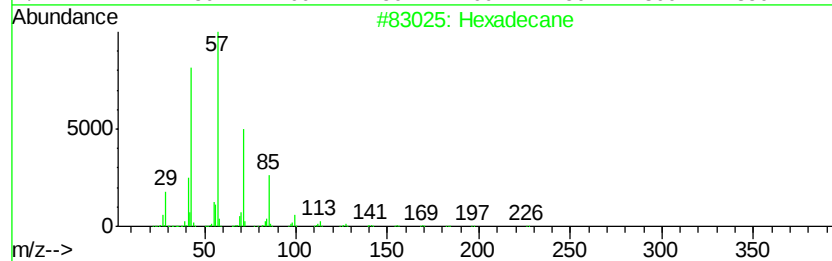
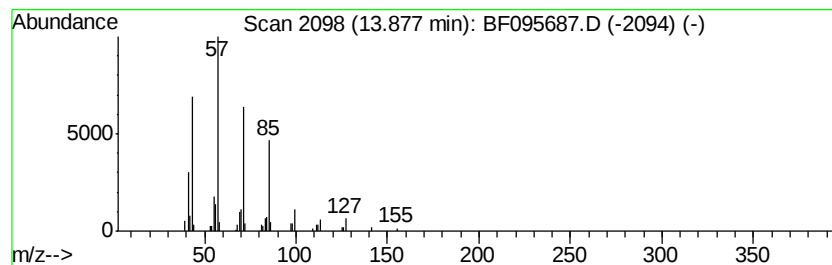
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.38 ng	148621	Phenanthrene-d10	14.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Tetradecane	198	C14H30	000629-59-4	86
3		Heptacosane	380	C27H56	000593-49-7	86
4		Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	78
5		Tritetracontane	605	C43H88	007098-21-7	78



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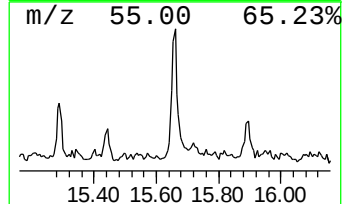
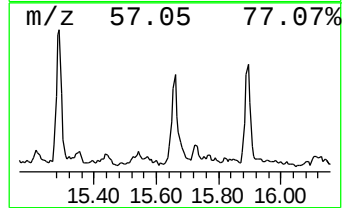
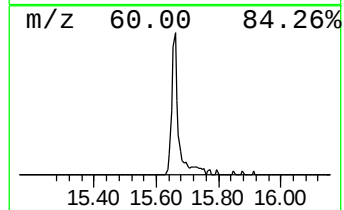
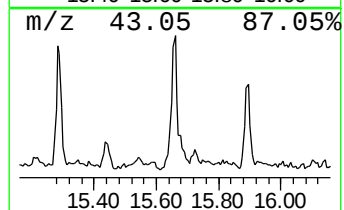
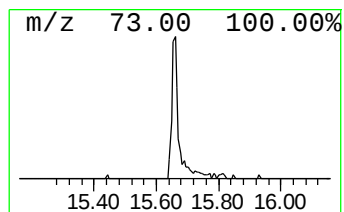
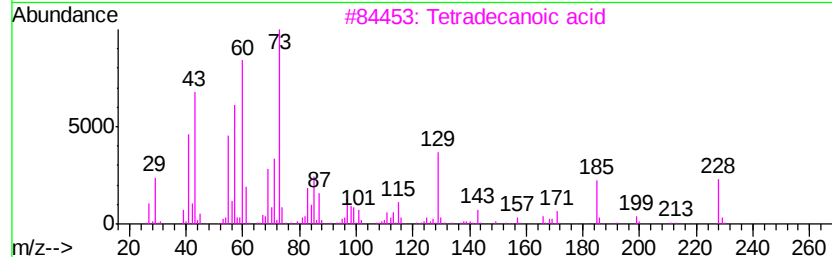
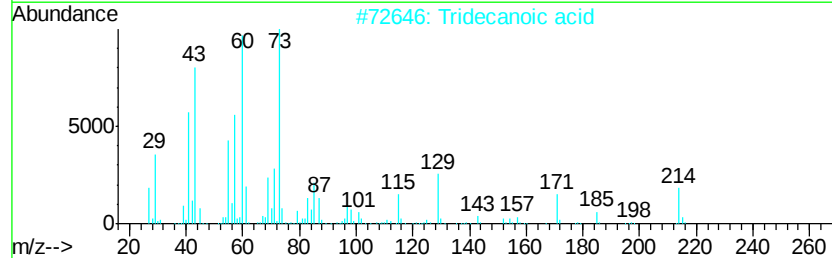
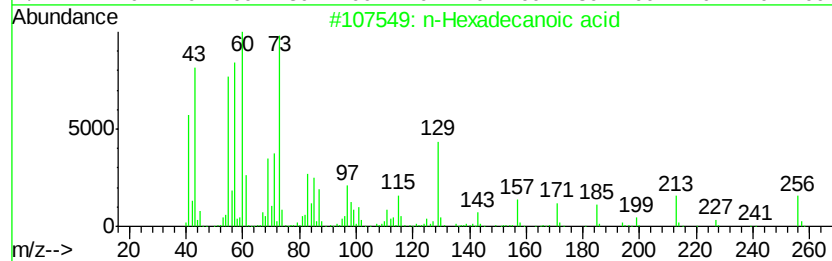
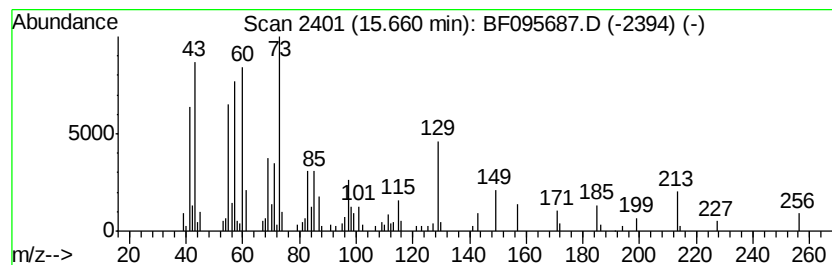
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.66	4.40 ng	193469	Phenanthrene-d10		14.64	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		Dodecanoic acid	200	C12H24O2	000143-07-7	68
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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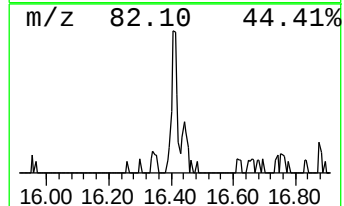
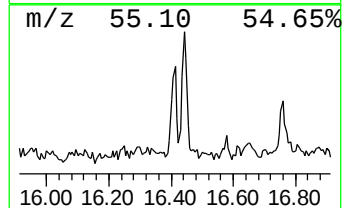
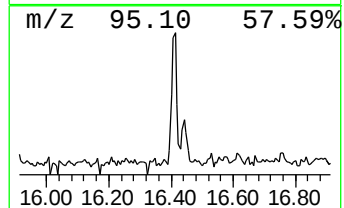
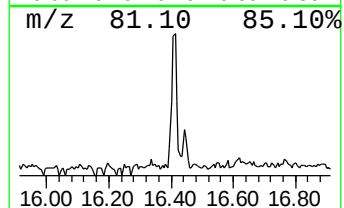
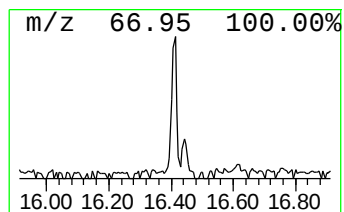
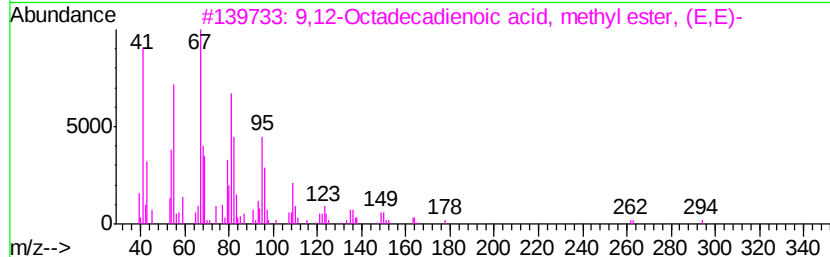
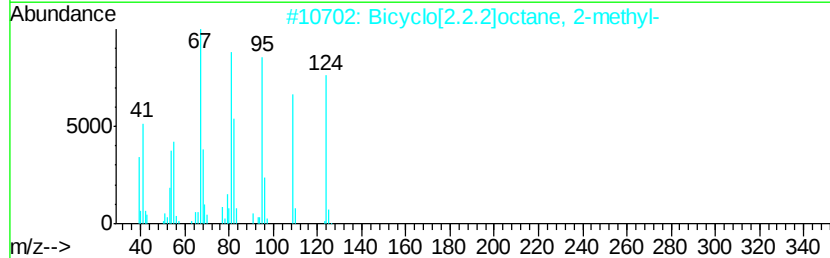
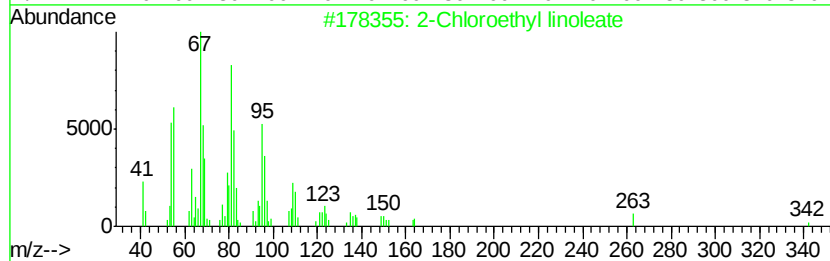
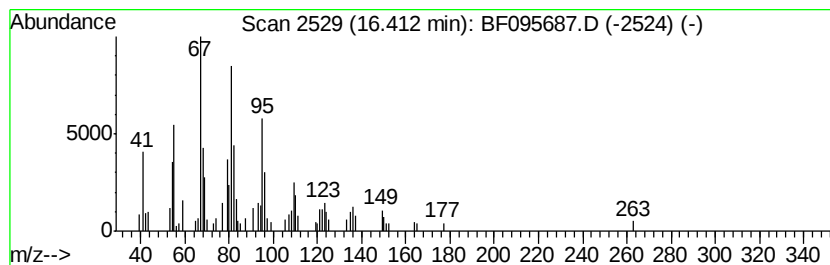
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Chloroethyl linoleate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.00 ng	88154	Phenanthrene-d10	14.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
2		Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	83
3		9,12-Octadecadienoic acid, methyl...	294	C19H34O2	002566-97-4	76
4		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	74
5		5-Undecyne	152	C11H20	002294-72-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
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Acq On : 5 Jun 2017 22:41
Operator : SJ/MA
Sample : I3438-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

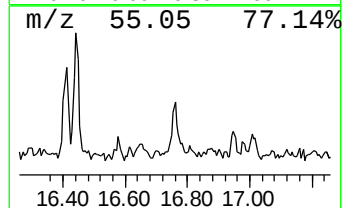
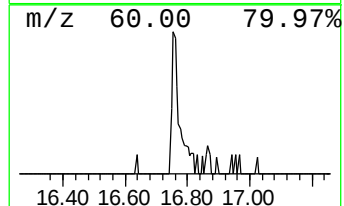
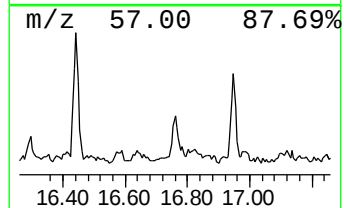
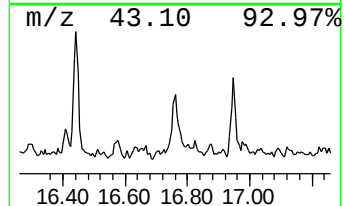
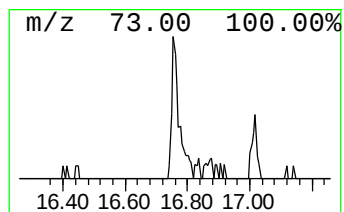
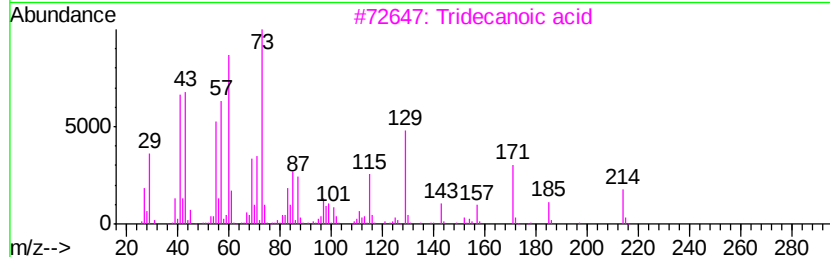
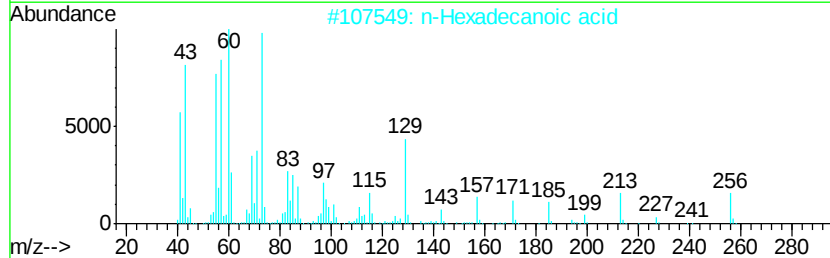
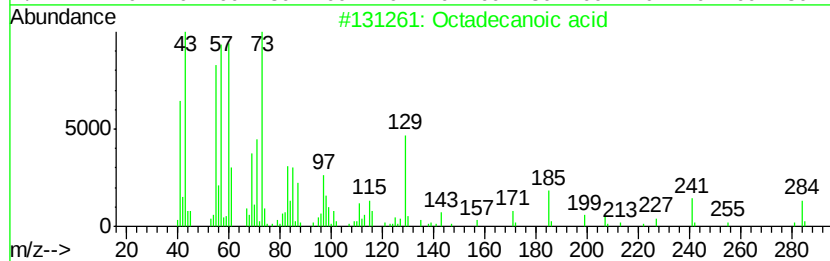
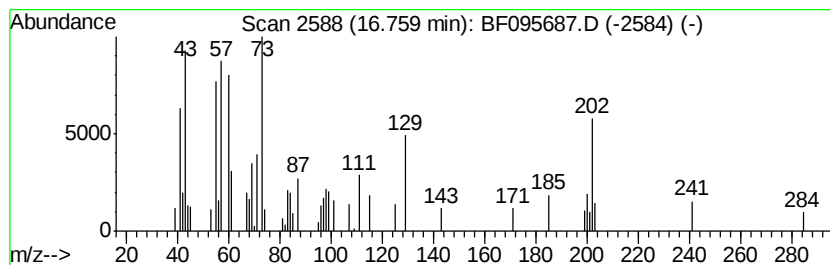
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ClientSampleId :
TP-8-9

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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 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.76	2.20 ng	60736	Chrysene-d12	18.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	50
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
3		Tridecanoic acid	214	C13H26O2	000638-53-9	47
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095687.D
Acq On : 5 Jun 2017 22:41
Operator : SJ/MA
Sample : I3438-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8-9

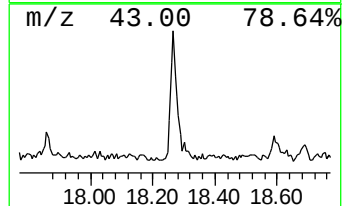
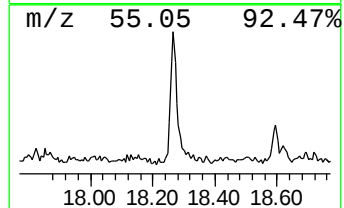
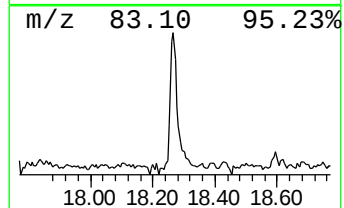
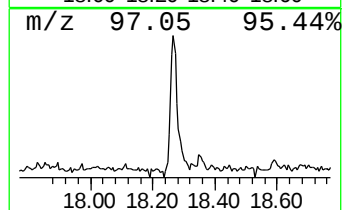
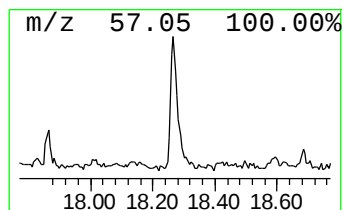
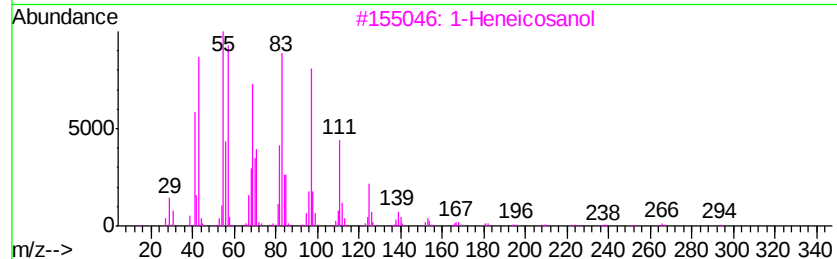
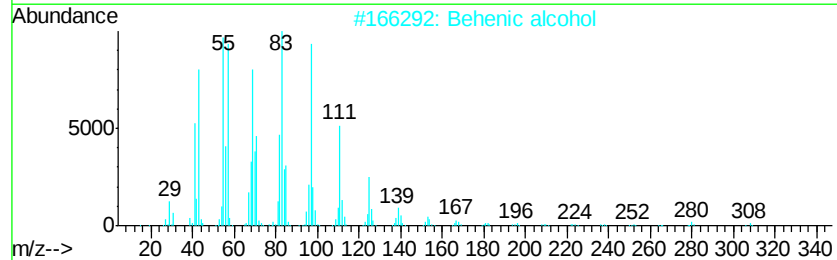
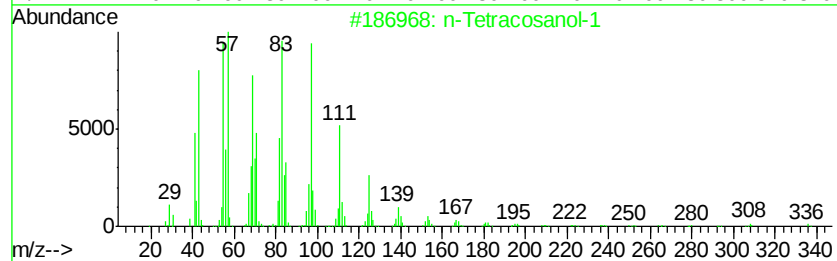
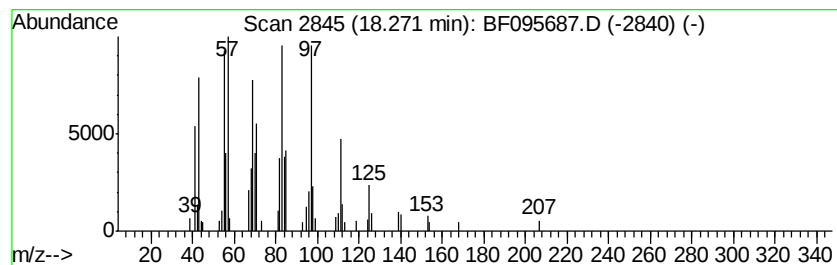
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	5.78 ng	159570	Chrysene-d12	18.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95



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Sample : I3438-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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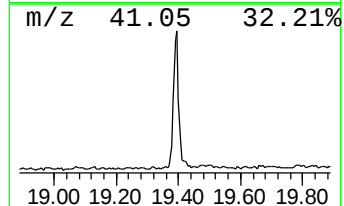
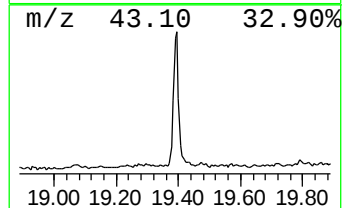
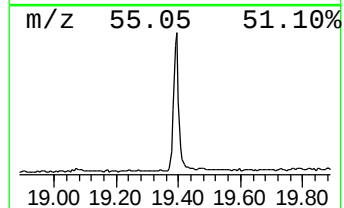
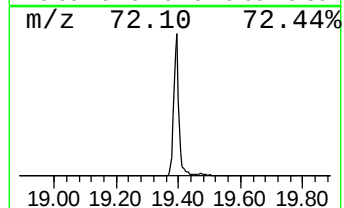
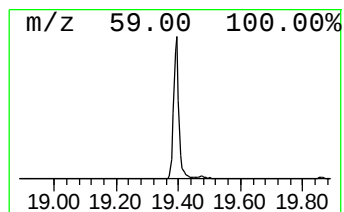
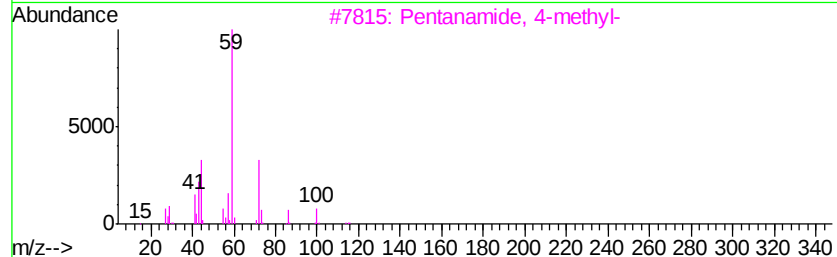
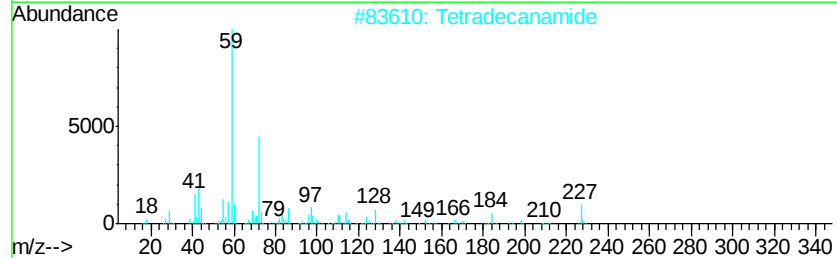
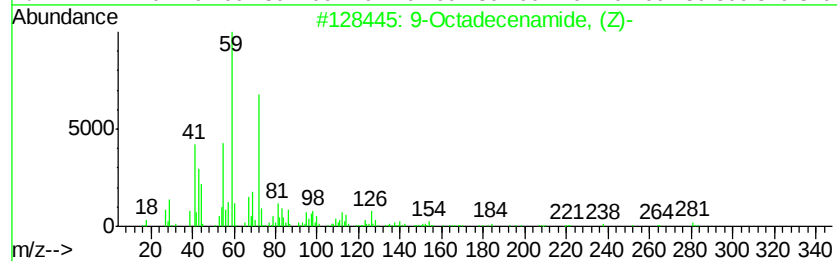
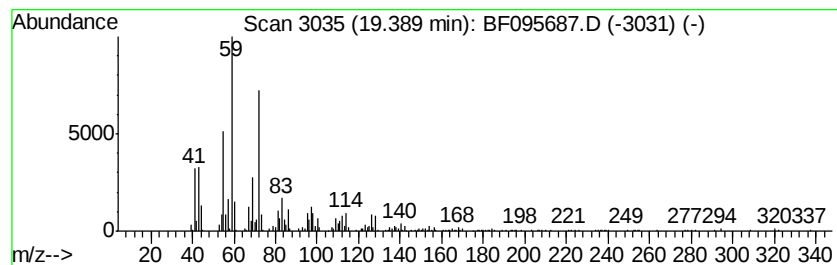
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	28.21 ng	780984	Perylene-d12	20.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Tetradecanamide	227	C14H29NO	000638-58-4	53
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	38
4		N,N-Dimethyl cyanoacetamide	112	C5H8N2O	007391-40-4	27
5		2,7-Dioxatricyclo[4.4.0.0(3,8)]d...	155	C8H13NO2	040076-28-6	27



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Acq On : 5 Jun 2017 22:41
Operator : SJ/MA
Sample : I3438-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.64	10.4	ng	302545	1	7.40	580242	20.0
unknown7.06	7.06	112.8	ng	3273050	1	7.40	580242	20.0
Hexadecane	13.11	2.0	ng	95364	3	12.25	949800	20.0
Tetradecane	13.88	3.4	ng	148621	4	14.64	880405	20.0
n-Hexadecanoic acid	15.66	4.4	ng	193469	4	14.64	880405	20.0
2-Chloroethyl lin...	16.41	2.0	ng	88154	4	14.64	880405	20.0
Octadecanoic acid	16.76	2.2	ng	60736	5	18.35	551884	20.0
n-Tetracosanol-1	18.27	5.8	ng	159570	5	18.35	551884	20.0
9-Octadecenamide, ...	19.39	28.2	ng	780984	6	20.02	553694	20.0