

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
 Data File : BF095042.D
 Acq On : 10 May 2017 2:00
 Operator : SJ/MA
 Sample : I3027-14
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7-8-9-COMP

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	4.113	366	370	385	rBV	60223	135855	4.29%	0.516%
2	5.042	524	528	546	rBV	207974	431488	13.62%	1.640%
3	5.672	630	635	666	rBV	1730865	2687752	84.84%	10.217%
4	7.266	901	906	920	rBV	1862850	2838095	89.58%	10.789%
5	7.378	920	925	945	rVB	2230038	3168138	100.00%	12.043%
6	7.713	978	982	994	rVB	495166	553467	17.47%	2.104%
7	7.954	1017	1023	1034	rBV	1877158	2293796	72.40%	8.720%
8	8.619	1130	1136	1155	rBV	1281366	1792881	56.59%	6.815%
9	9.730	1321	1325	1345	rBV	562480	734464	23.18%	2.792%
10	11.507	1621	1627	1646	rBV	2332039	2955046	93.27%	11.233%
11	12.201	1741	1745	1756	rBV	165814	222251	7.02%	0.845%
12	12.560	1801	1806	1819	rBV2	530395	796080	25.13%	3.026%
13	13.401	1943	1949	1956	rBV	43551	50938	1.61%	0.194%
14	13.860	2021	2027	2048	rBV	1198949	1797625	56.74%	6.833%
15	14.177	2076	2081	2084	rBV	49269	65528	2.07%	0.249%
16	14.906	2200	2205	2210	rBV	28265	36316	1.15%	0.138%
17	14.959	2210	2214	2230	rVB2	480037	696813	21.99%	2.649%
18	15.930	2373	2379	2387	rBV2	113066	144849	4.57%	0.551%
19	17.018	2560	2564	2570	rBV2	46478	64631	2.04%	0.246%
20	17.130	2579	2583	2589	rVB	33385	36846	1.16%	0.140%
21	17.289	2604	2610	2614	rBV	2003287	2283570	72.08%	8.681%
22	17.959	2720	2724	2725	rBV	98104	104526	3.30%	0.397%
23	17.983	2725	2728	2739	rVV	930793	1027899	32.44%	3.907%
24	18.089	2742	2746	2755	rVB	43685	57220	1.81%	0.218%
25	18.536	2818	2822	2831	rBV3	33002	54177	1.71%	0.206%
26	18.630	2834	2838	2845	rBV	428198	511544	16.15%	1.945%
27	19.653	3008	3012	3016	rBV	47580	59922	1.89%	0.228%
28	20.300	3117	3122	3133	rBV	347765	511664	16.15%	1.945%
29	20.394	3134	3138	3143	rVB2	33279	48660	1.54%	0.185%
30	20.765	3197	3201	3205	rVB3	40329	62032	1.96%	0.236%
31	21.188	3270	3273	3276	rBV2	29952	40106	1.27%	0.152%
32	21.683	3353	3357	3362	rVB2	27112	42117	1.33%	0.160%

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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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

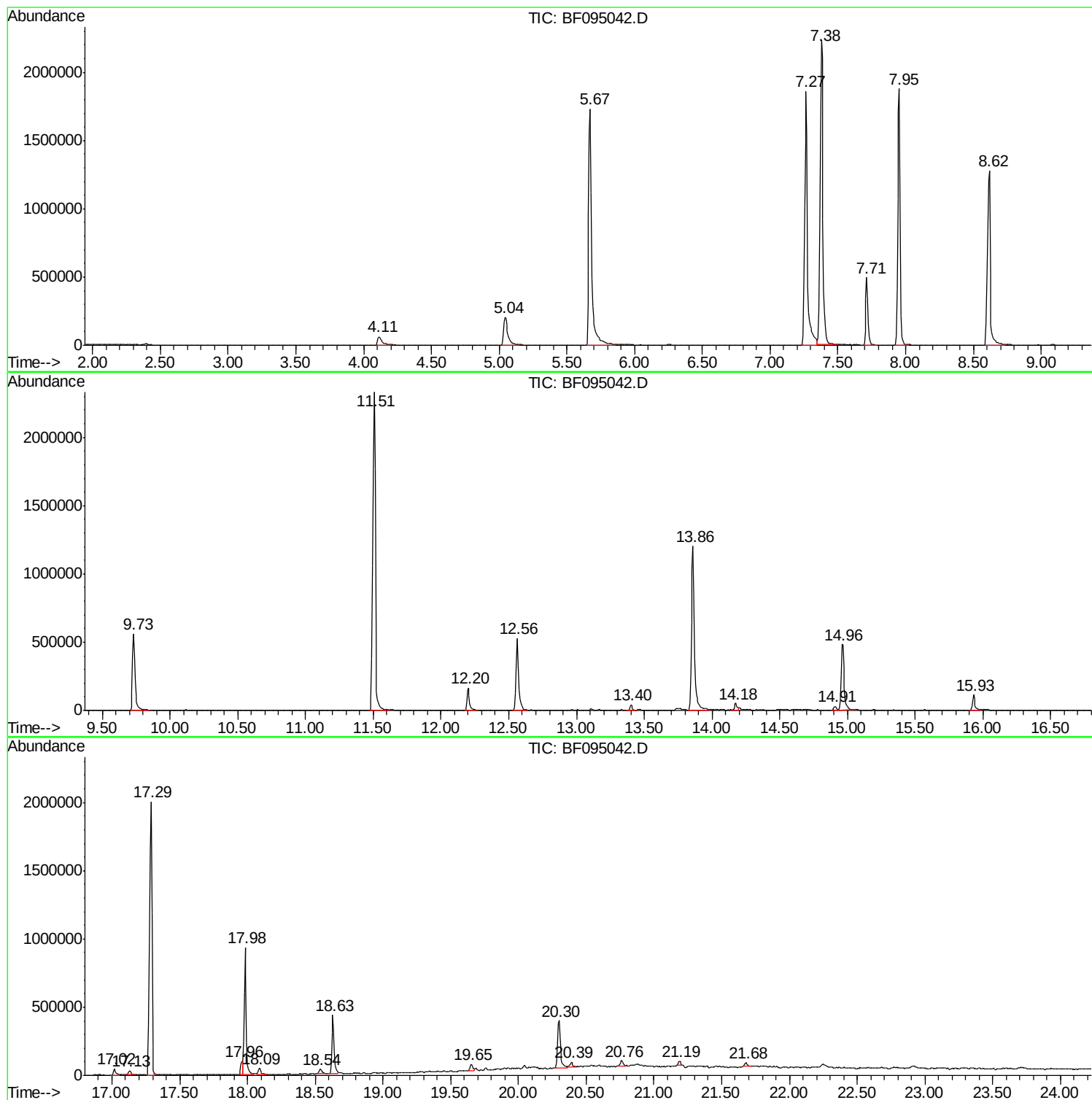
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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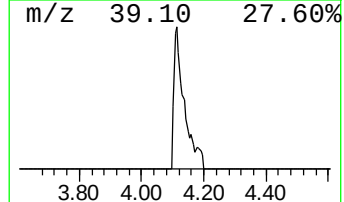
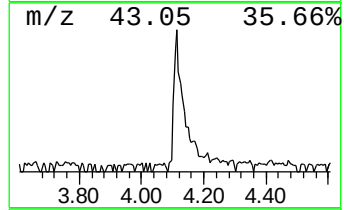
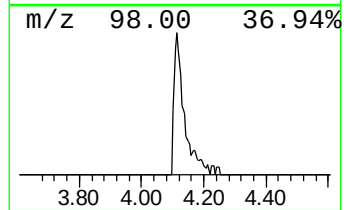
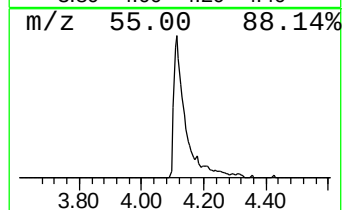
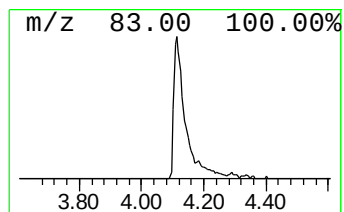
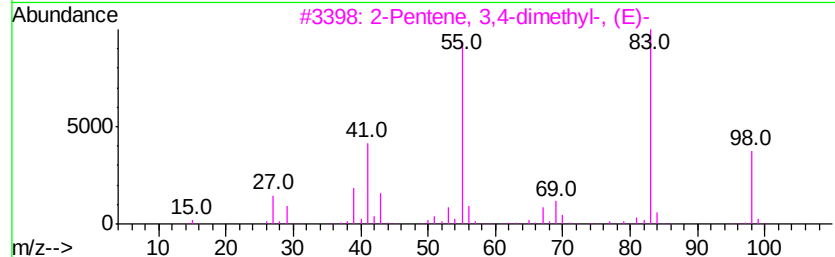
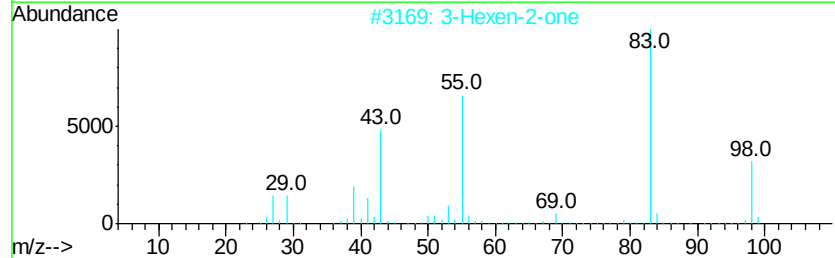
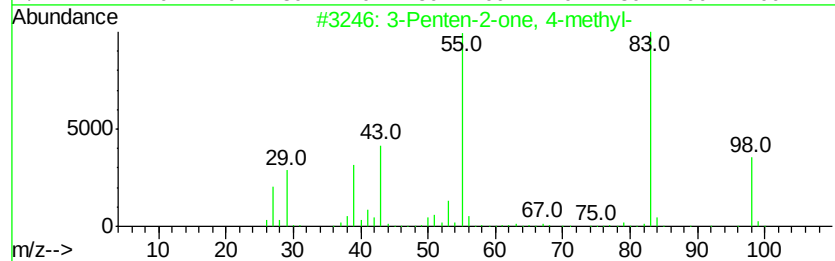
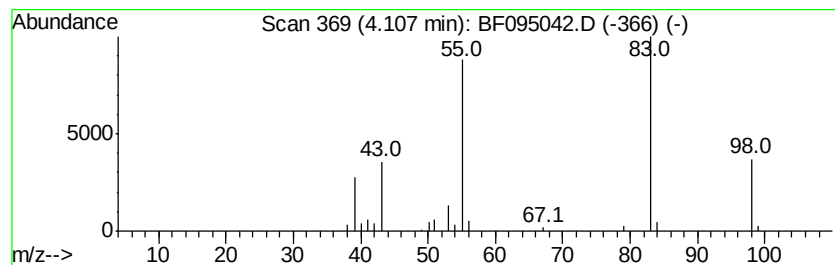
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	4.91 ng	135855	1,4-Dichlorobenzene-d4	7.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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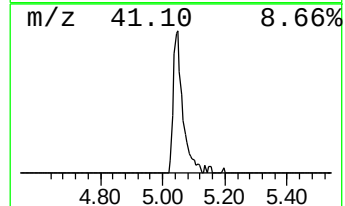
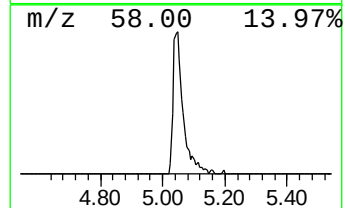
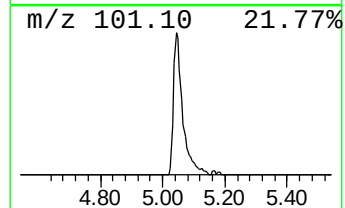
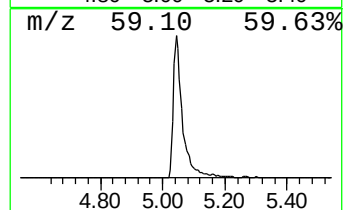
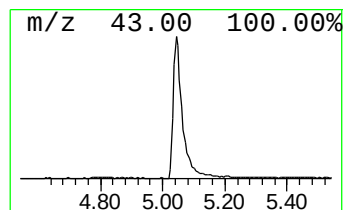
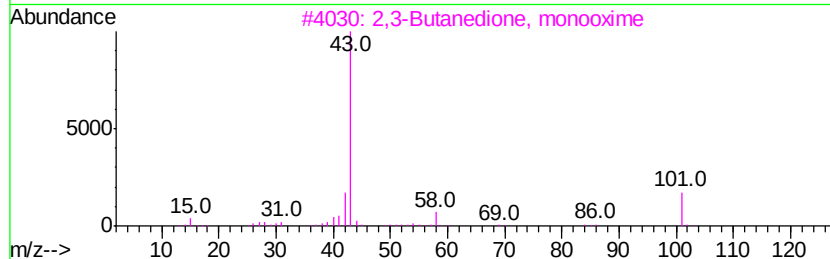
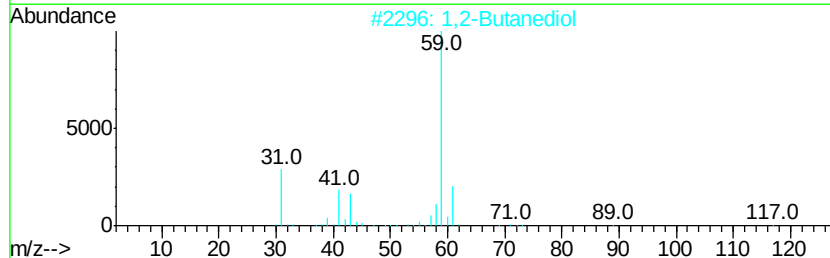
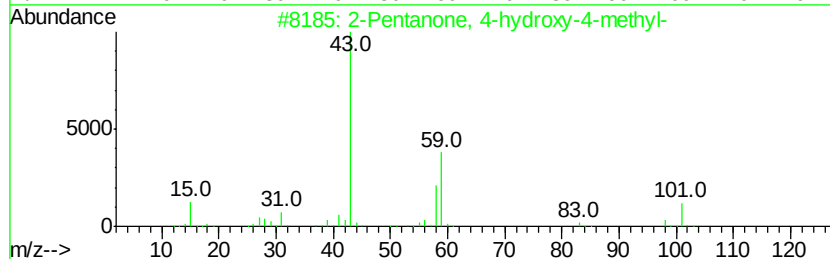
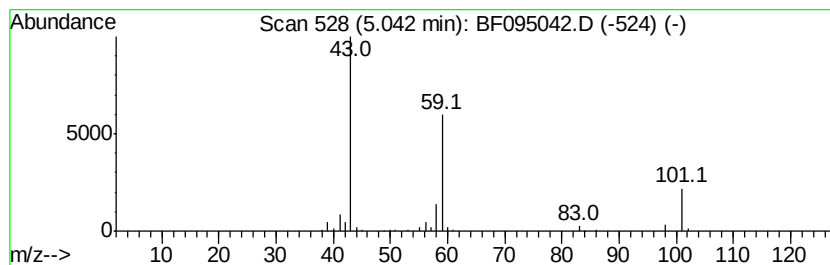
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	15.59 ng	431488	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,2-Butanediol	90	C4H10O2	000584-03-2	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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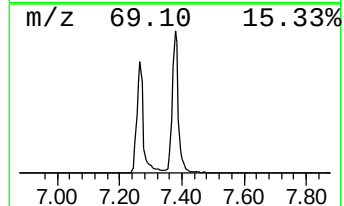
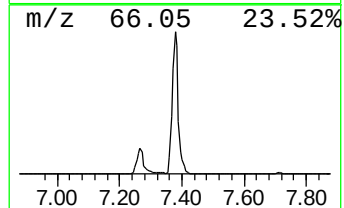
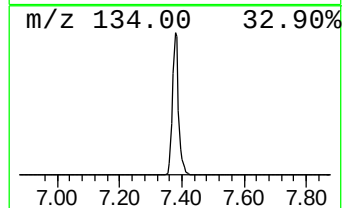
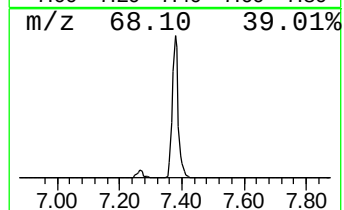
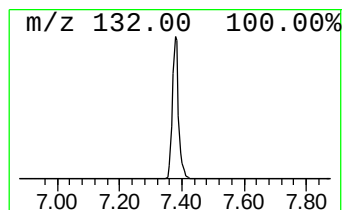
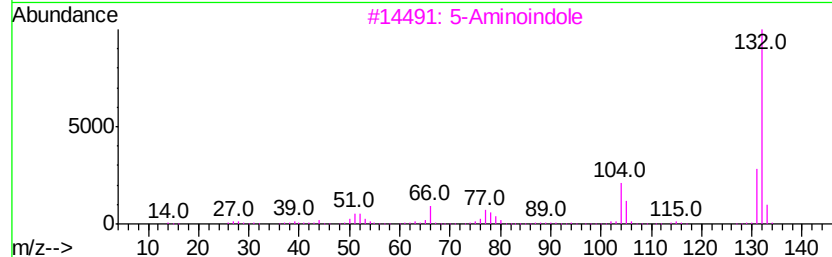
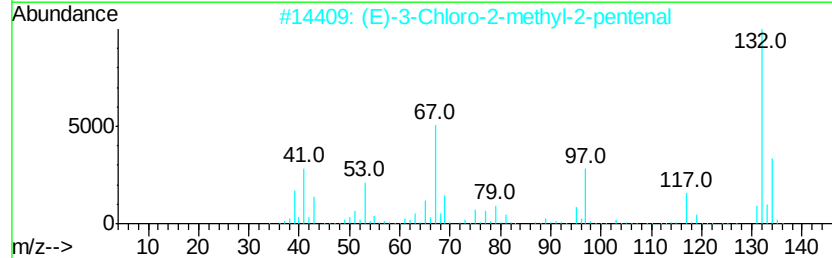
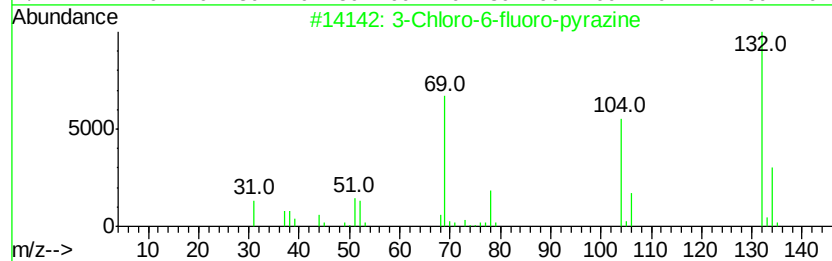
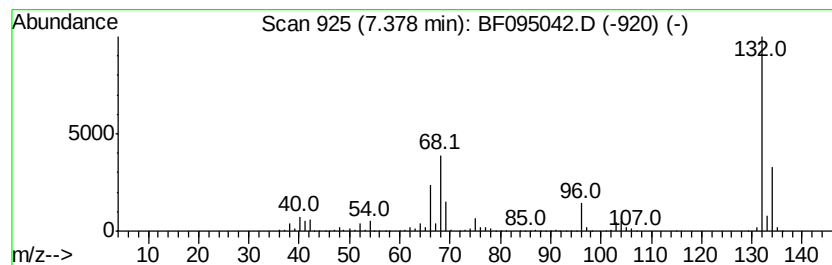
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	114.48 ng	3168140	1,4-Dichlorobenzene-d4	7.71

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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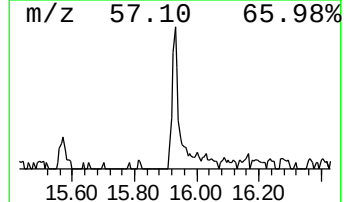
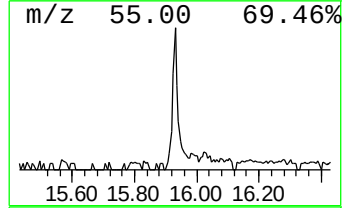
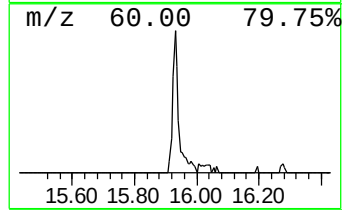
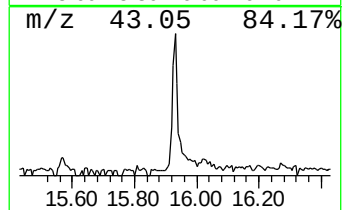
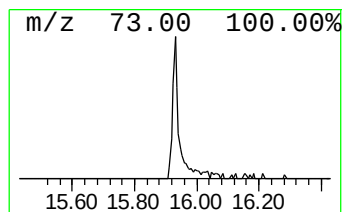
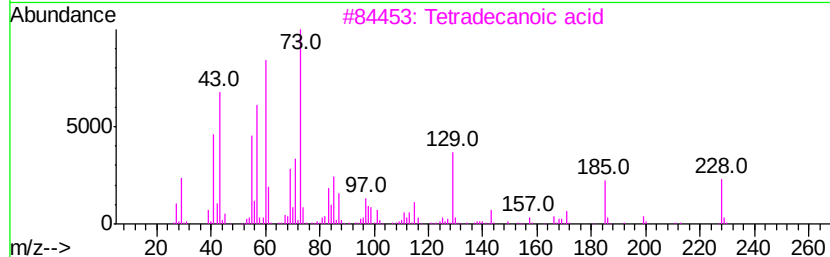
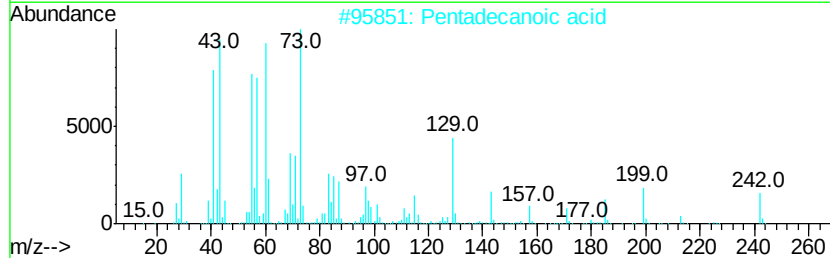
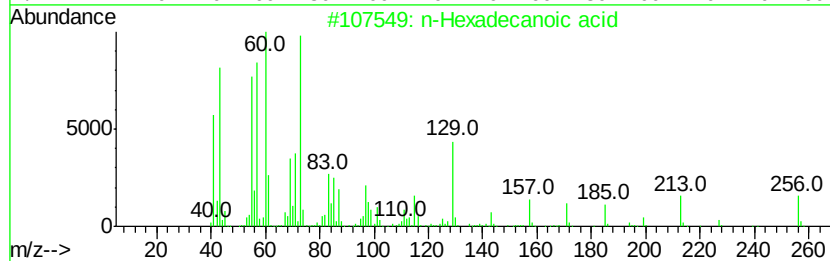
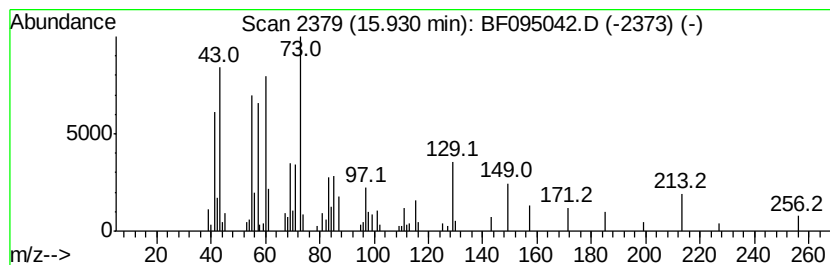
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.16 ng	144849	Phenanthrene-d10	14.96

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	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Dodecanoic acid	200	C12H24O2	000143-07-7	52



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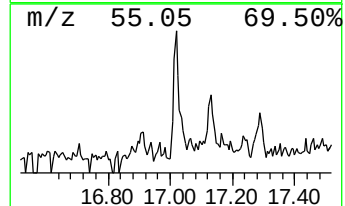
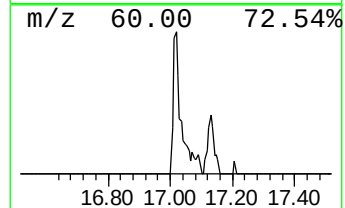
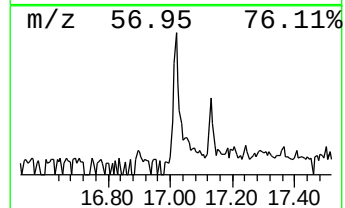
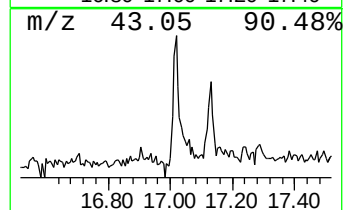
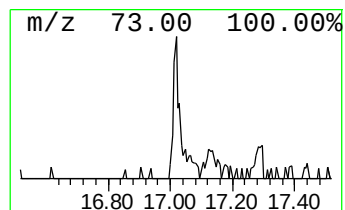
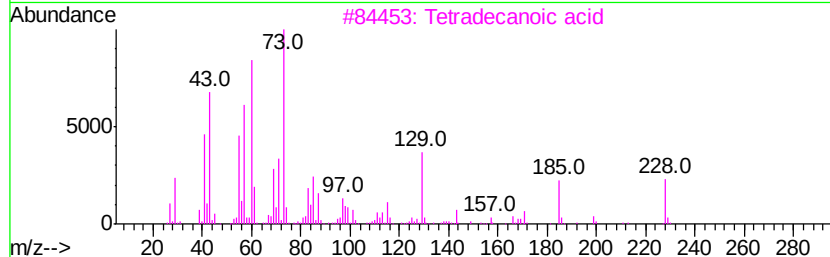
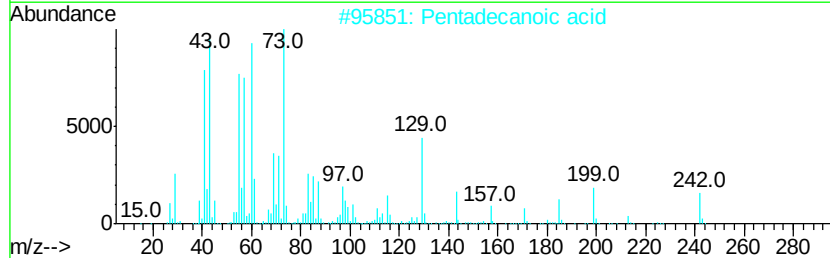
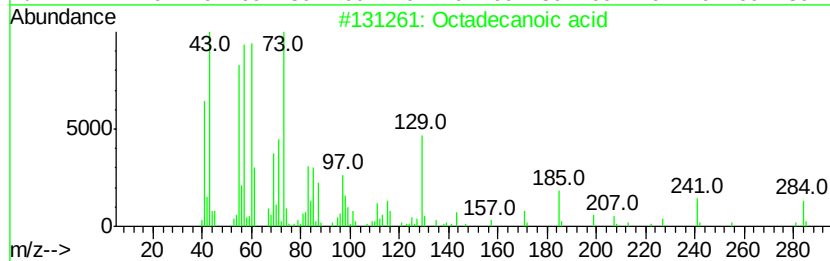
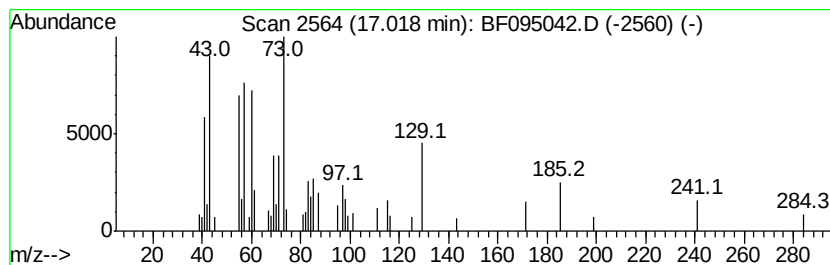
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	2.53 ng	64631	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	27



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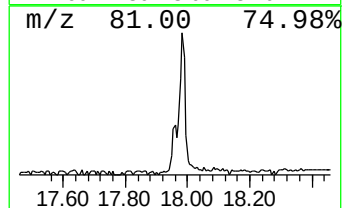
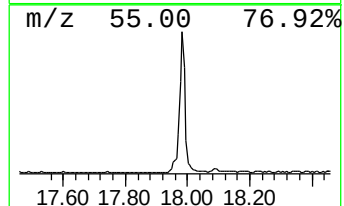
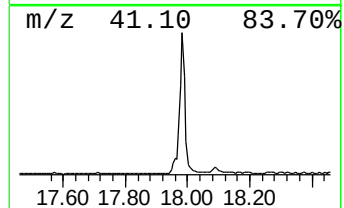
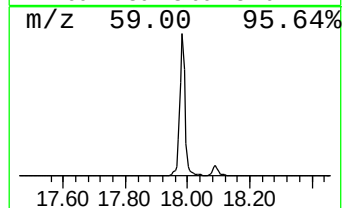
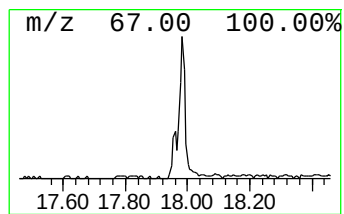
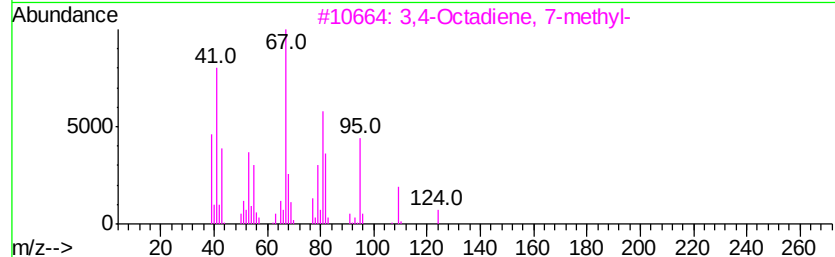
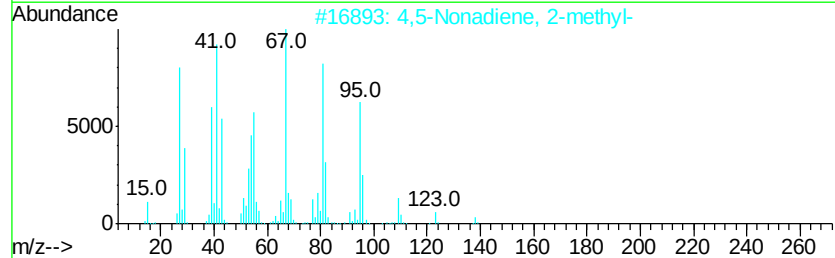
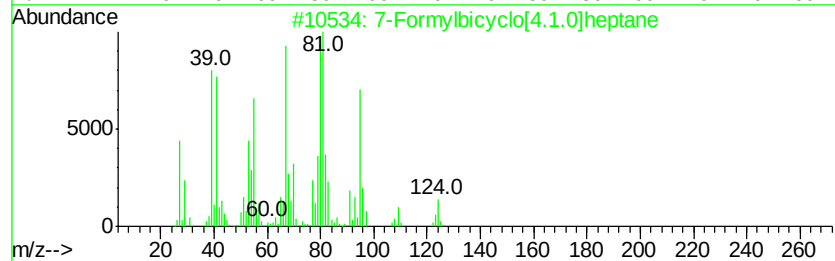
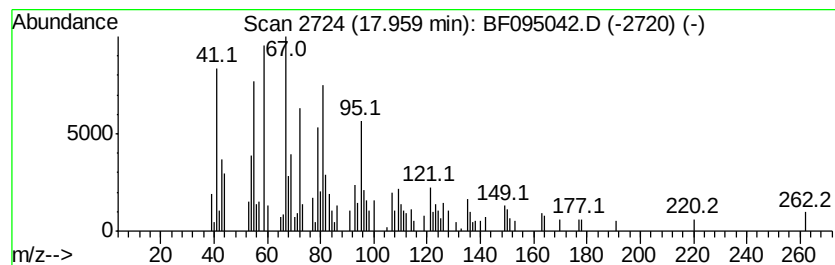
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TP-7-8-9-COMP

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 7-Formylbicyclo[4.1.0]heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.96	4.09 ng	104526	Chrysene-d12	18.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Formylbicyclo[4.1.0]heptane	124	C8H12O	1000197-01-8	55
2	4,5-Nonadiene, 2-methyl-	138	C10H18	055956-32-6	49
3	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	49
4	4-Tetradecyne	194	C14H26	060212-33-1	46
5	8-Hexadecyne	222	C16H30	019781-86-3	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095042.D
Acq On : 10 May 2017 2:00
Operator : SJ/MA
Sample : I3027-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7-8-9-COMP

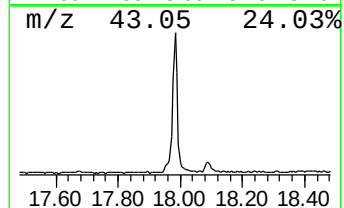
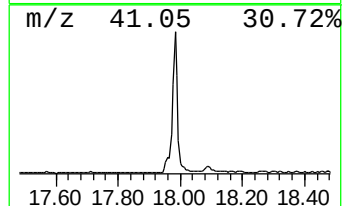
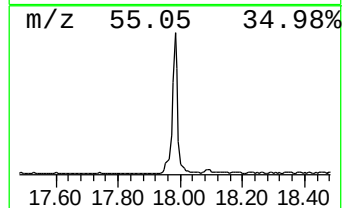
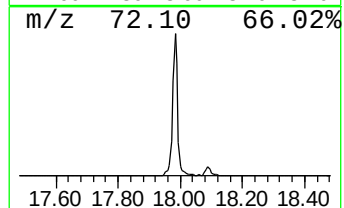
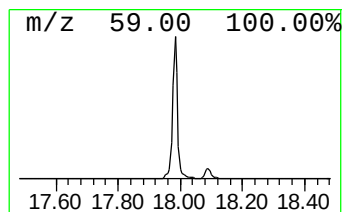
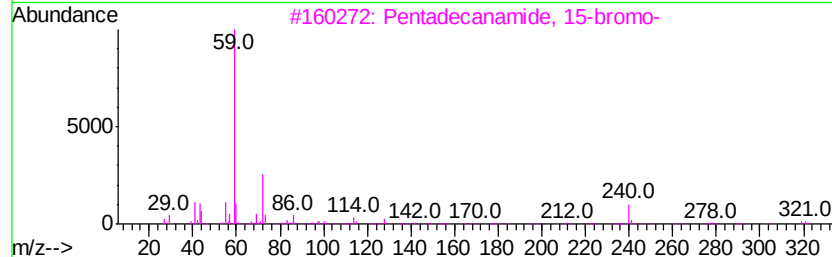
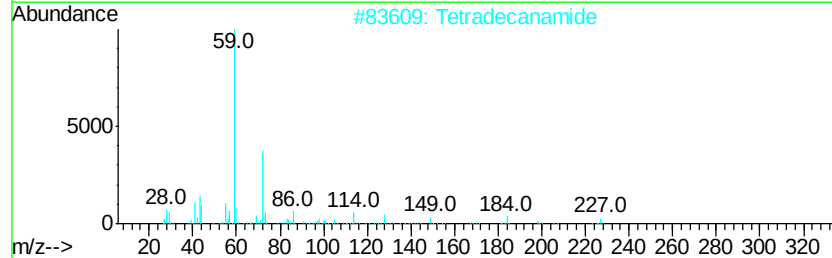
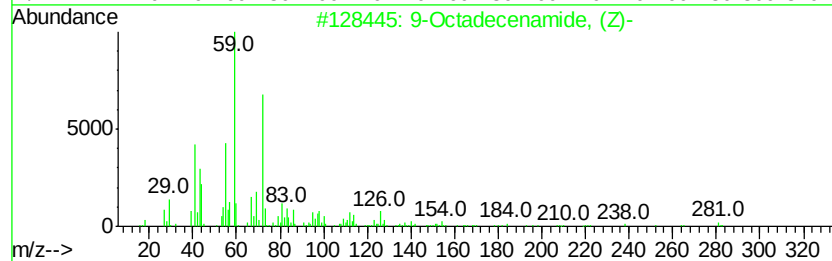
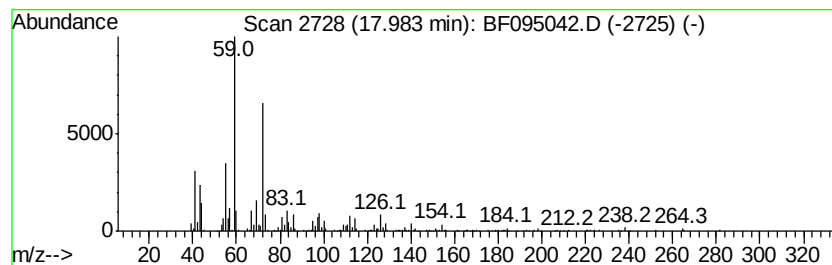
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	40.19 ng	1027900	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Tetradecanamide	227	C14H29NO	000638-58-4	72
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	56
4		Hexadecanamide	255	C16H33NO	000629-54-9	56
5		Nonanamide	157	C9H19NO	001120-07-6	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095042.D
Acq On : 10 May 2017 2:00
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-7-8-9-COMP

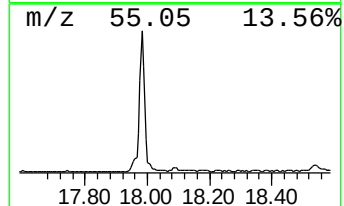
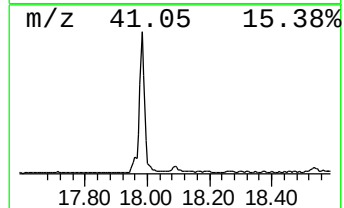
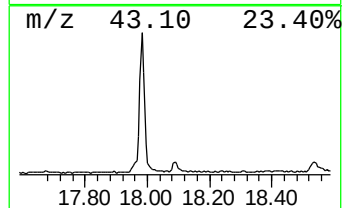
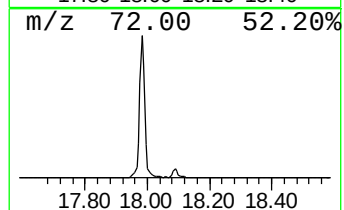
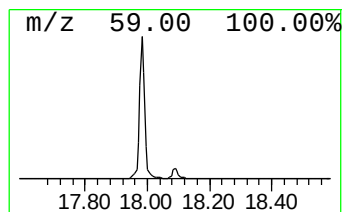
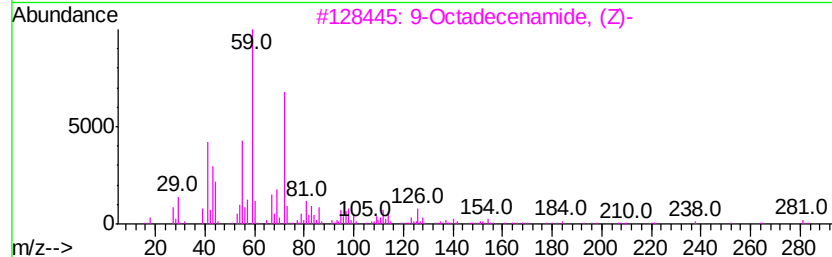
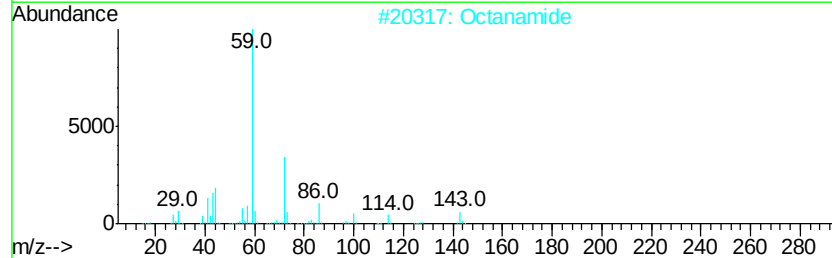
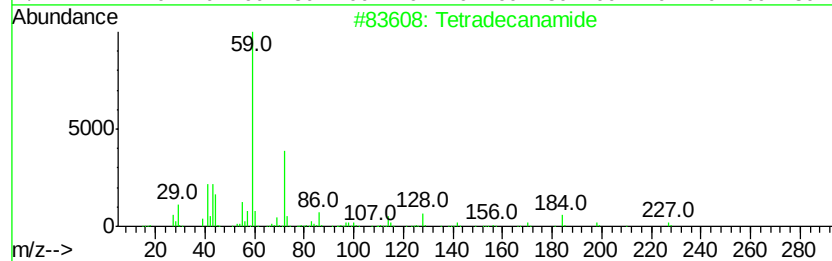
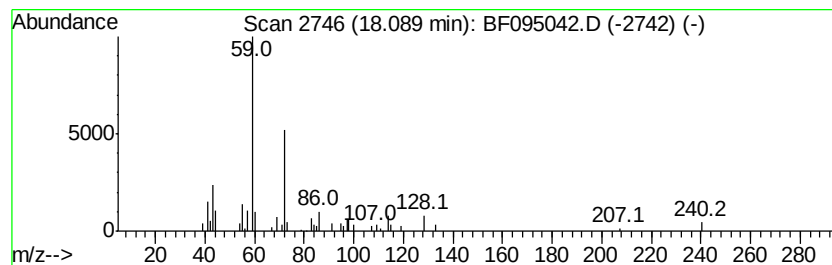
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	2.24 ng	57220	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanamide	227	C14H29NO	000638-58-4	64
2		Octanamide	143	C8H17NO	000629-01-6	64
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Decanamide-	171	C10H21NO	002319-29-1	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095042.D
Acq On : 10 May 2017 2:00
Operator : SJ/MA
Sample : I3027-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

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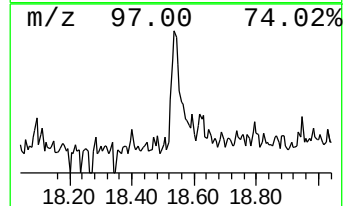
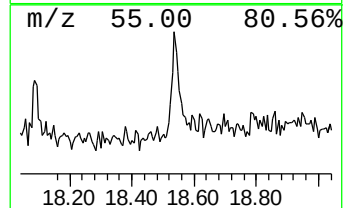
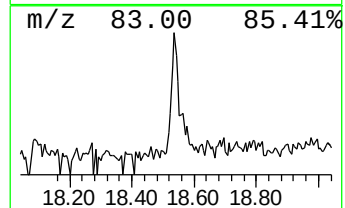
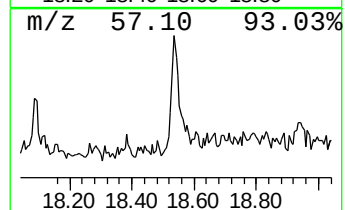
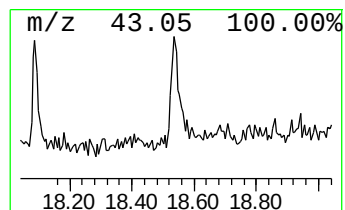
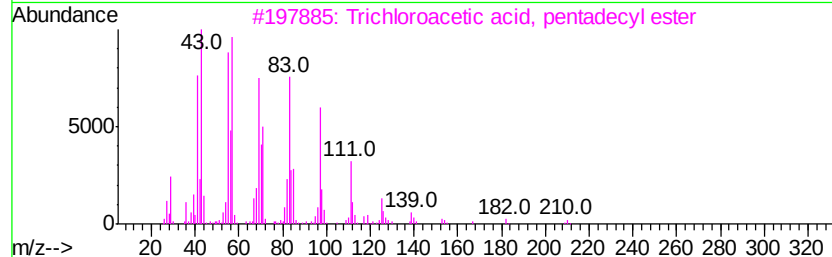
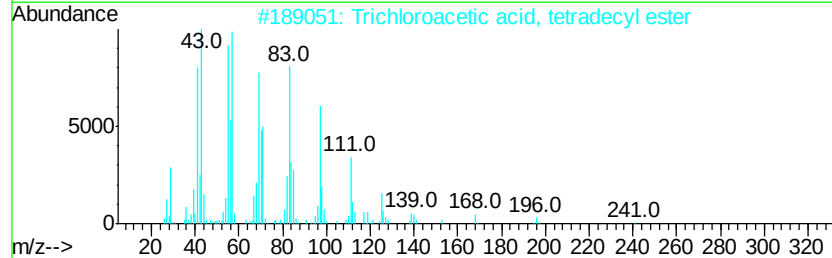
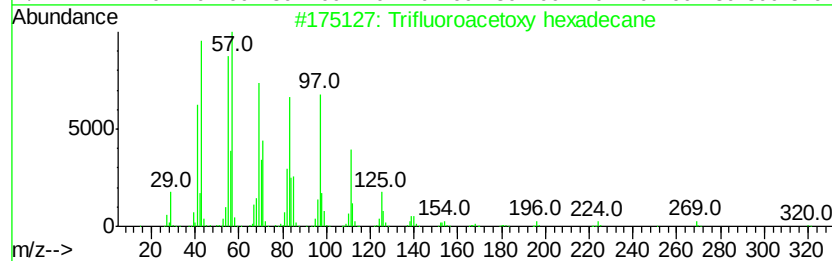
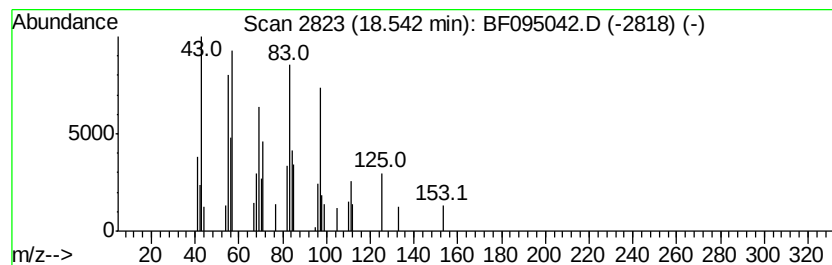
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	2.12 ng	54177	Chrysene-d12	18.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	87
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095042.D
Acq On : 10 May 2017 2:00
Operator : SJ/MA
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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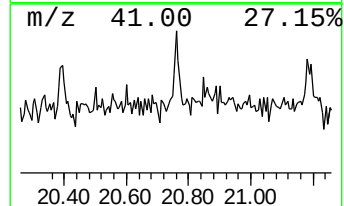
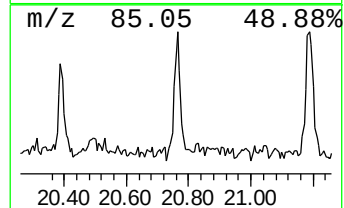
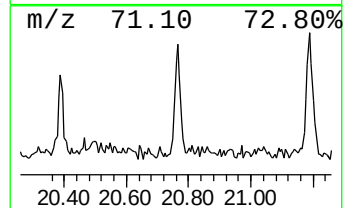
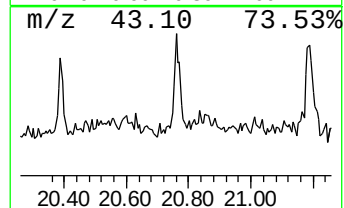
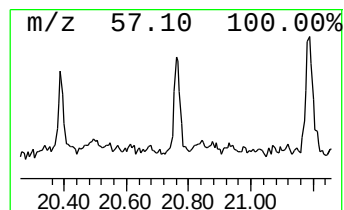
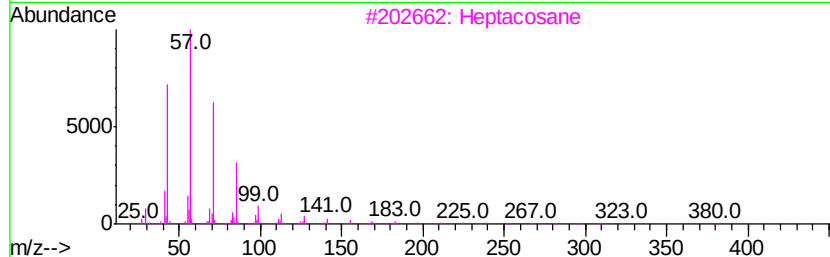
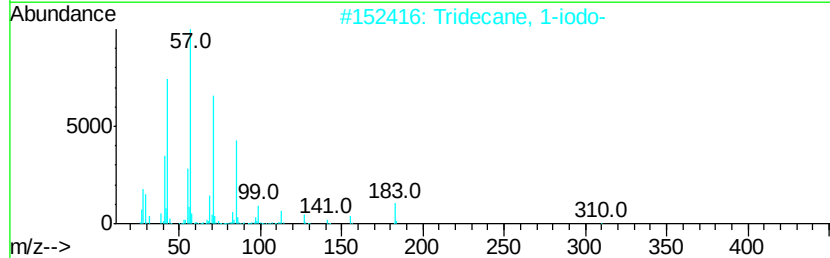
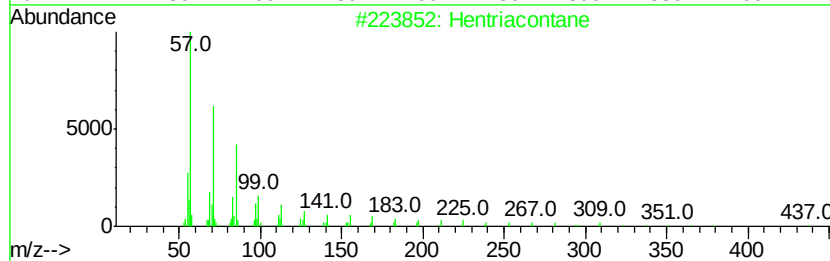
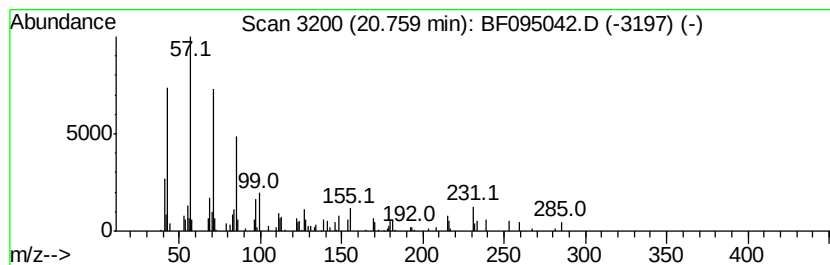
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	2.42 ng	62032	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	72
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59
3		Heptacosane	380	C27H56	000593-49-7	59
4		Tridecane, 6-propyl-	226	C16H34	055045-10-8	53
5		Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
Data File : BF095042.D
Acq On : 10 May 2017 2:00
Operator : SJ/MA
Sample : I3027-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.04	15.6	ng	431488	1	7.71	553467	20.0
unknown7.38	7.38	114.5	ng	3168140	1	7.71	553467	20.0
n-Hexadecanoic acid	15.93	4.2	ng	144849	4	14.96	696813	20.0
Octadecanoic acid	17.02	2.5	ng	64631	5	18.63	511544	20.0
7-Formylbicyclo[4...	17.96	4.1	ng	104526	5	18.63	511544	20.0
9-Octadecenamide,...	17.98	40.2	ng	1027900	5	18.63	511544	20.0
Tetradecanamide	18.09	2.2	ng	57220	5	18.63	511544	20.0
Trifluoroacetoxy ...	18.54	2.1	ng	54177	5	18.63	511544	20.0
Hentriacontane	20.76	2.4	ng	62032	6	20.30	511664	20.0