

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
 Data File : BF099188.D
 Acq On : 7 Oct 2017 12:21
 Operator : SJ/JU
 Sample : I5585-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G69-1.5-3

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-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	2.169	9	14	22	rVB	149737	195173	5.23%	0.609%
2	2.993	145	154	164	rBV	42550	68202	1.83%	0.213%
3	4.475	402	406	414	rBV	102627	117654	3.15%	0.367%
4	5.098	508	512	526	rVB	420524	603376	16.17%	1.882%
5	5.492	574	579	582	rBV	2981443	3359895	90.06%	10.479%
6	6.504	745	751	754	rBV	2922148	3367682	90.27%	10.503%
7	6.639	769	774	777	rBV	3390382	3438184	92.16%	10.723%
8	6.863	808	812	815	rBV	990488	788936	21.15%	2.461%
9	7.022	834	839	842	rBV	2947444	2727991	73.12%	8.508%
10	7.434	903	909	911	rBV	1967989	2217915	59.45%	6.917%
11	8.145	1026	1030	1033	rBV	1320001	1051934	28.20%	3.281%
12	9.222	1207	1213	1216	rBV	3900596	3730865	100.00%	11.636%
13	9.610	1276	1279	1282	rBV	577546	427381	11.46%	1.333%
14	9.898	1324	1328	1332	rBV2	1265747	1082417	29.01%	3.376%
15	10.322	1397	1400	1402	rVB	59491	45337	1.22%	0.141%
16	10.692	1458	1463	1466	rBV	1986299	1907965	51.14%	5.951%
17	10.792	1477	1480	1485	rBV	71456	74564	2.00%	0.233%
18	11.386	1577	1581	1584	rBV	1195947	991450	26.57%	3.092%
19	11.904	1663	1669	1673	rBV3	112819	122058	3.27%	0.381%
20	12.774	1813	1817	1821	rBV3	63384	72531	1.94%	0.226%
21	12.845	1821	1829	1839	rVV	371670	630104	16.89%	1.965%
22	12.968	1845	1850	1854	rBV	2699381	2751540	73.75%	8.582%
23	13.439	1925	1930	1936	rBV	307415	295399	7.92%	0.921%
24	13.851	1997	2000	2008	rBV2	87636	99021	2.65%	0.309%
25	14.021	2025	2029	2033	rBV	727897	695215	18.63%	2.168%
26	15.121	2213	2216	2220	rVB	34879	37823	1.01%	0.118%
27	15.498	2275	2280	2292	rBV	585977	771818	20.69%	2.407%
28	15.933	2350	2354	2360	rVB	65402	92347	2.48%	0.288%
29	16.439	2435	2440	2446	rBV	66228	115026	3.08%	0.359%
30	17.033	2536	2541	2548	rVB2	47254	96950	2.60%	0.302%
31	17.727	2654	2659	2668	rVB5	39554	86345	2.31%	0.269%

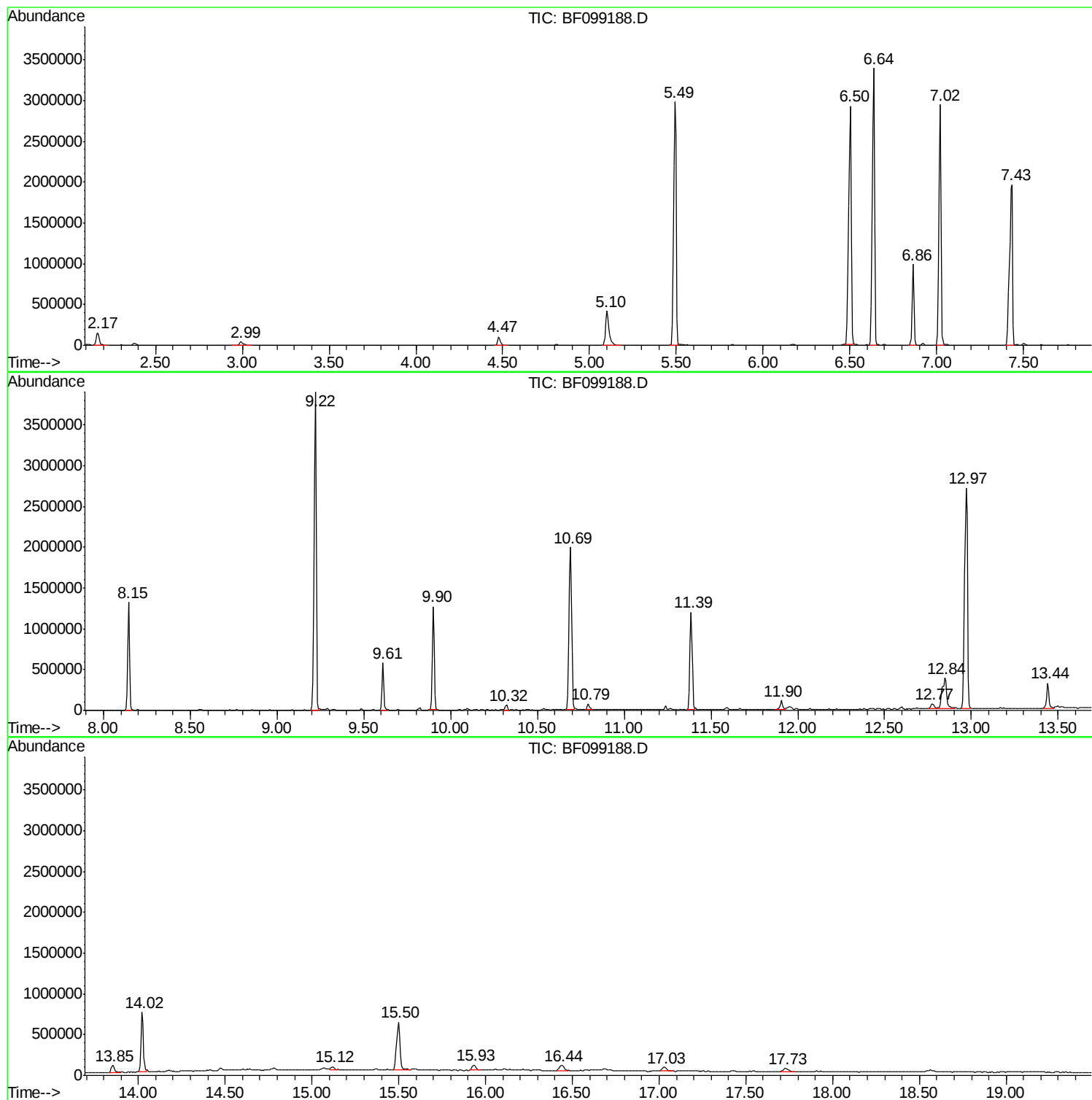
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ClientSampled :
G69-1.5-3

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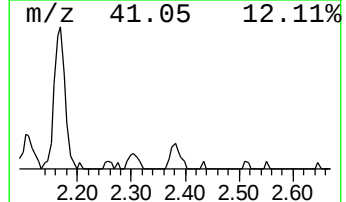
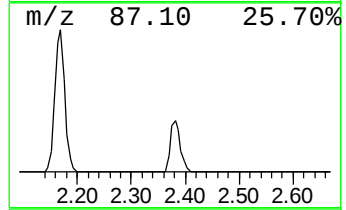
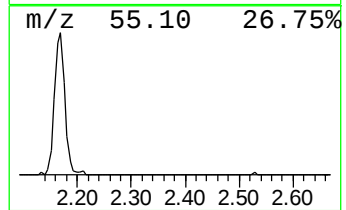
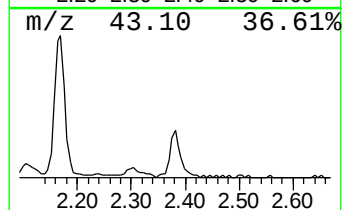
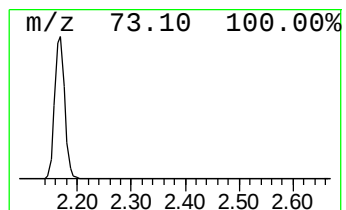
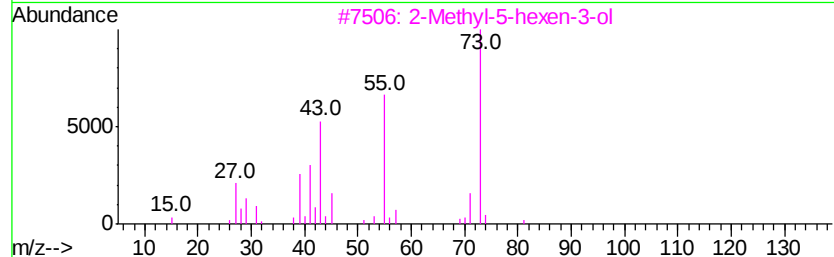
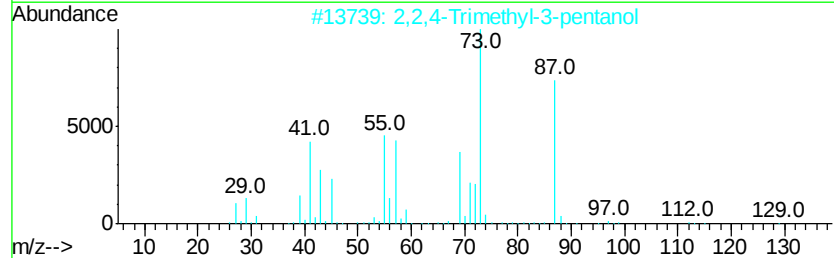
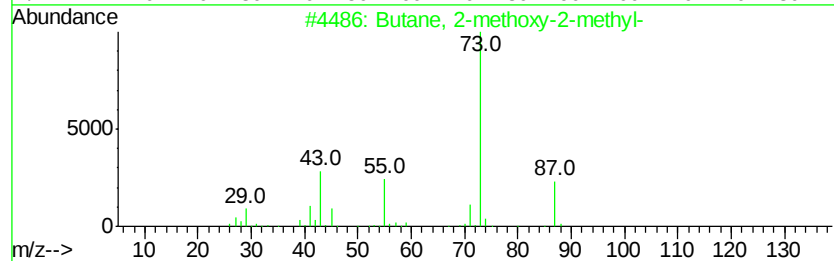
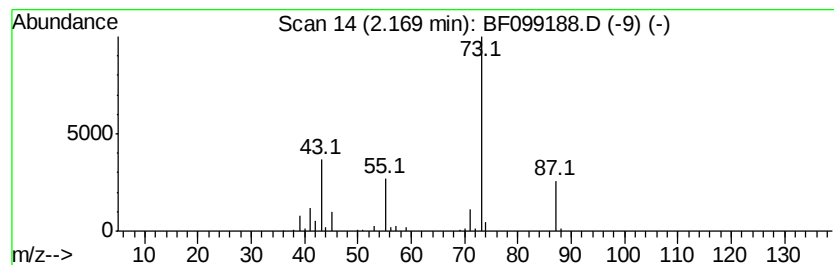
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	4.95 ng	195173	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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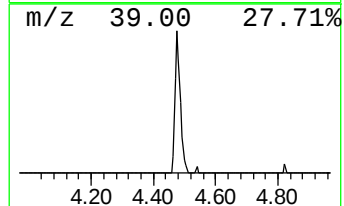
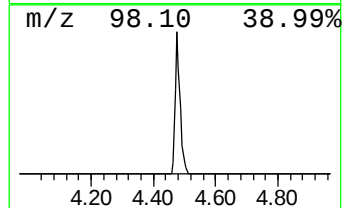
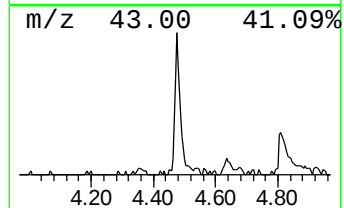
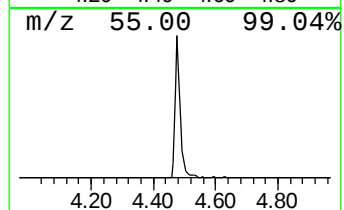
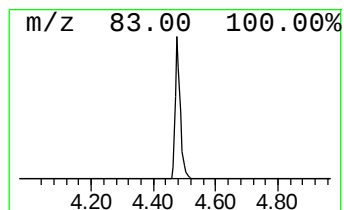
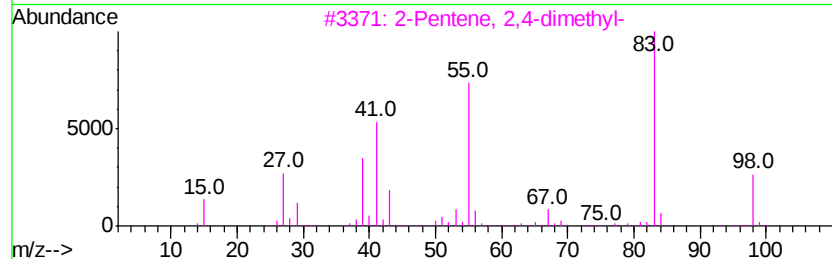
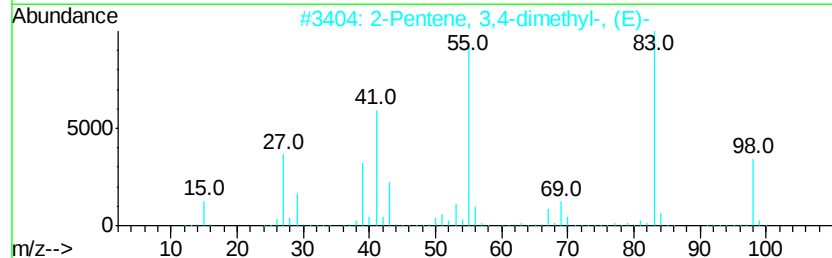
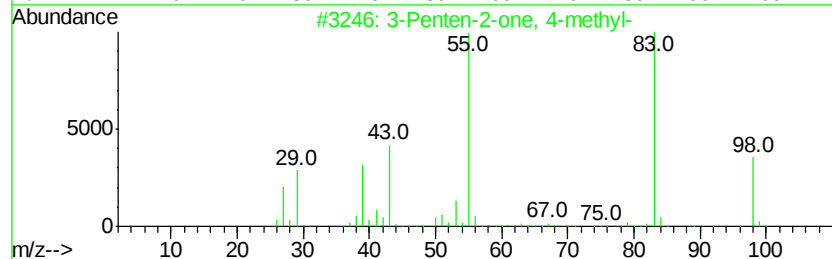
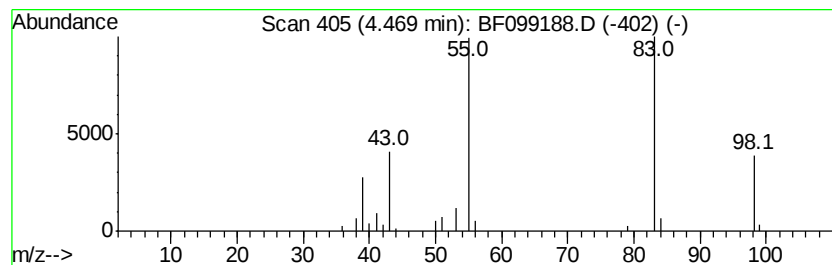
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TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	2.98 ng	117654	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4			3-Hexen-2-one	98	C6H10O	000763-93-9	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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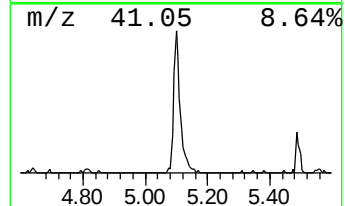
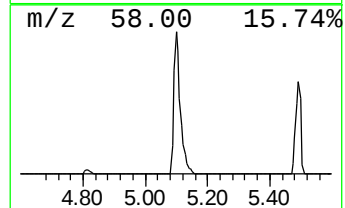
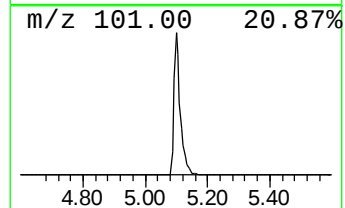
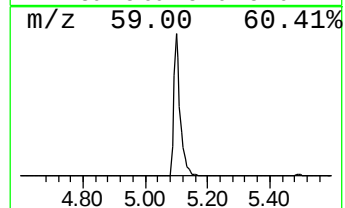
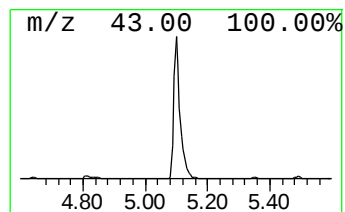
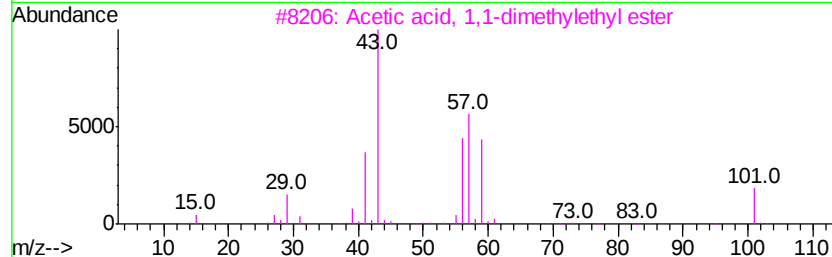
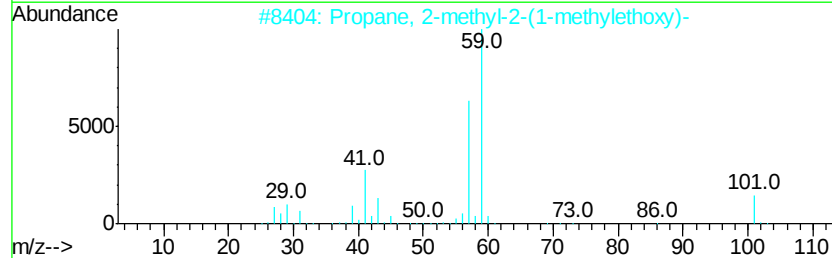
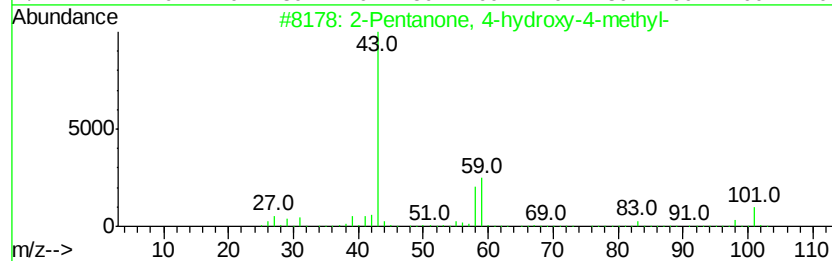
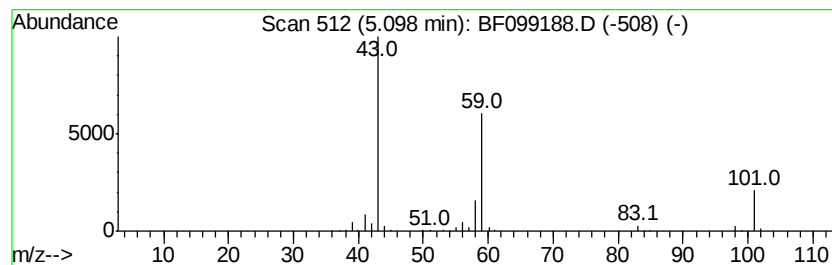
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	15.30 ng	603376	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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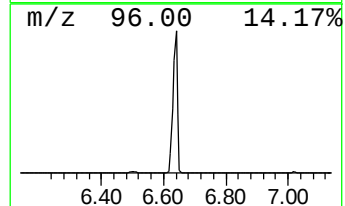
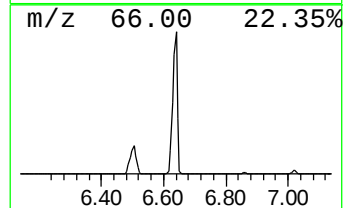
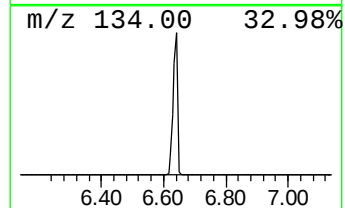
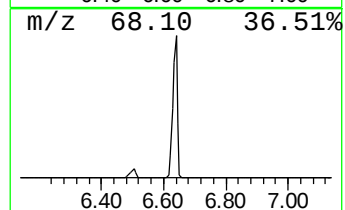
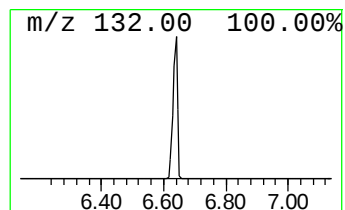
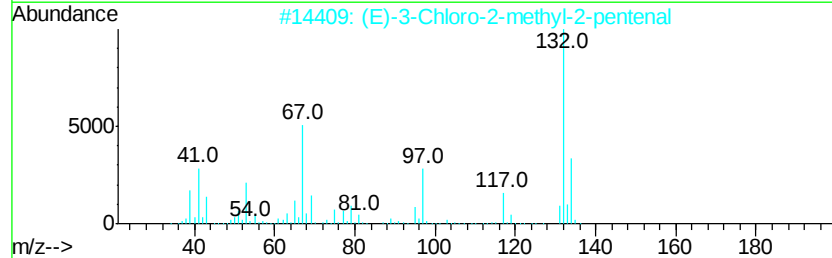
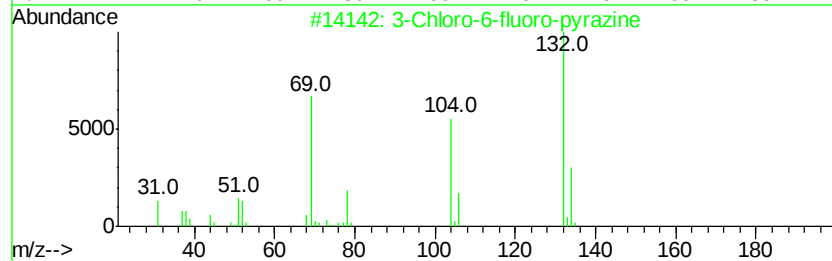
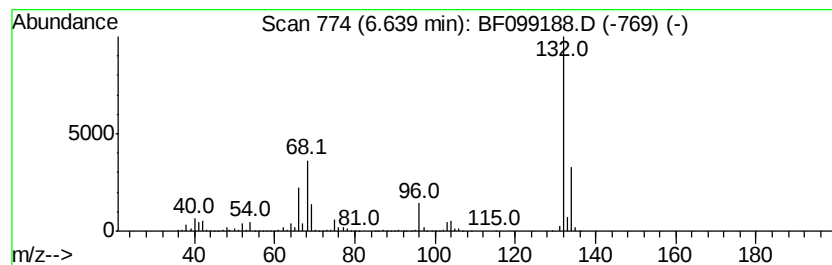
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	87.16 ng	3438180	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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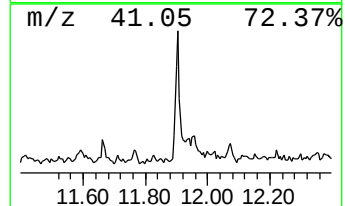
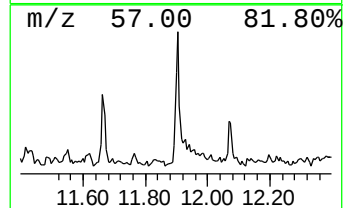
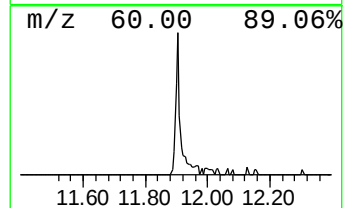
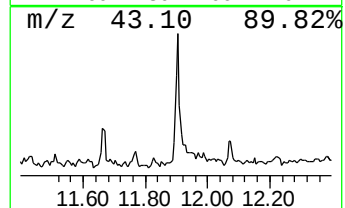
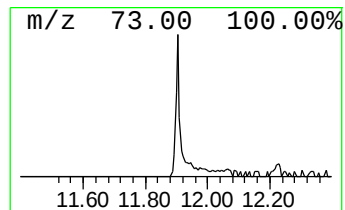
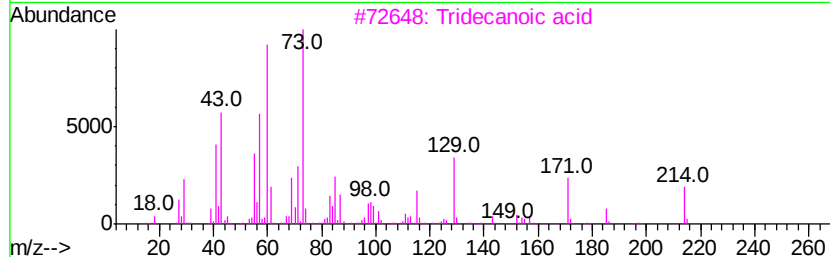
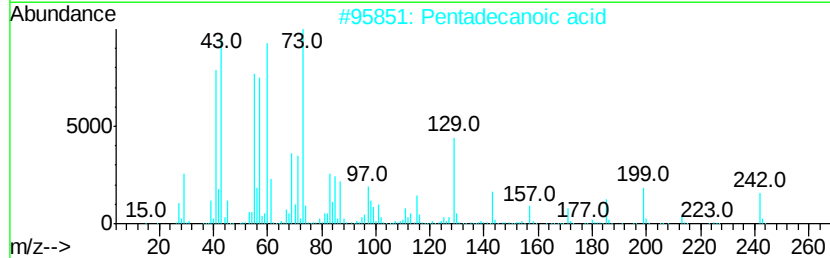
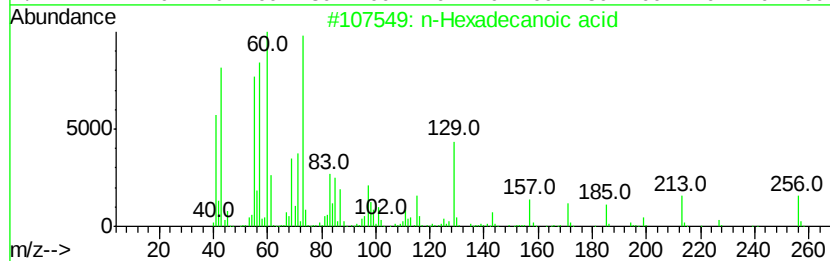
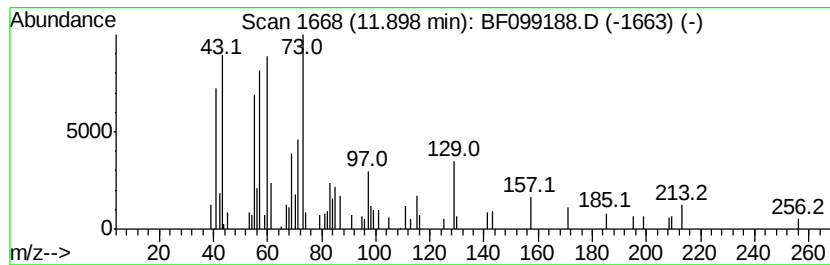
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.46 ng	122058	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20



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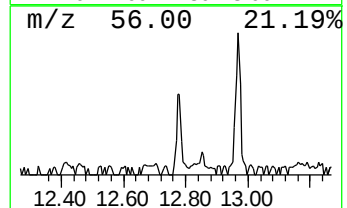
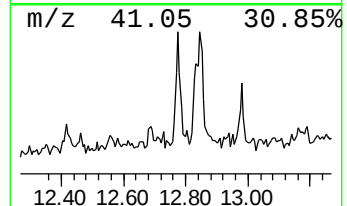
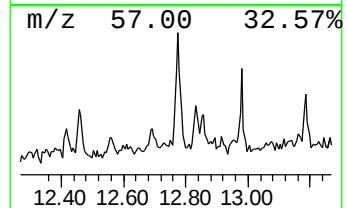
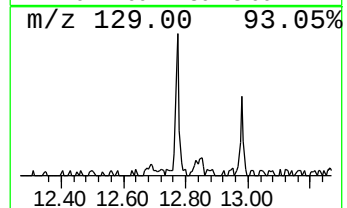
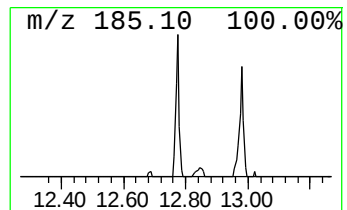
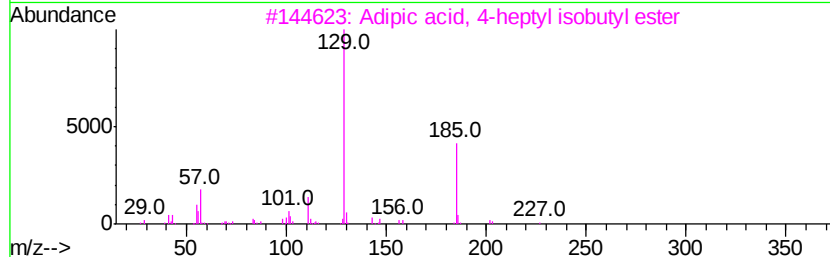
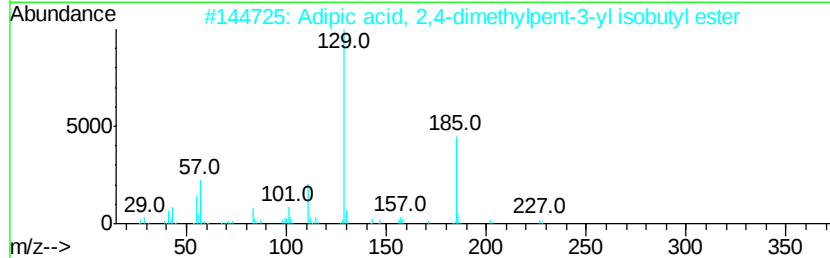
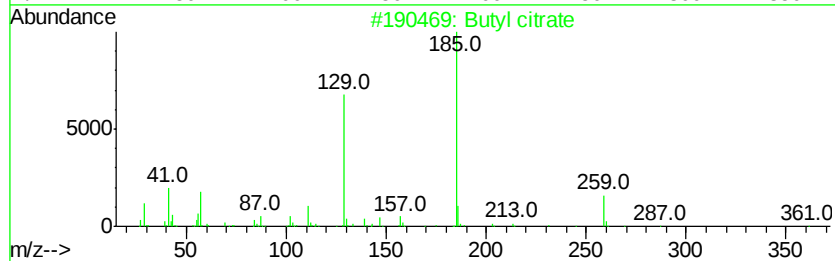
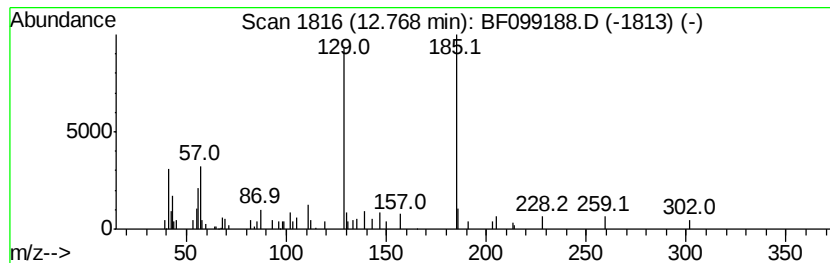
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ClientSampleId :
G69-1.5-3

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

Peak Number 7 Butyl citrate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.09 ng	72531	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	64
2	Adipic acid, 2,4-dimethylpent-3-...	300 C17H32O4	1000349-77-6	64
3	Adipic acid, 4-heptyl isobutyl e...	300 C17H32O4	1000349-73-6	59
4	Adipic acid, butyl pent-4-en-2-y...	270 C15H26O4	1000354-11-9	59
5	Adipic acid, isobutyl 2-pentyl e...	272 C15H28O4	1000324-15-6	56



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099188.D
Acq On : 7 Oct 2017 12:21
Operator : SJ/JU
Sample : I5585-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

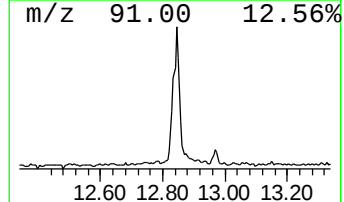
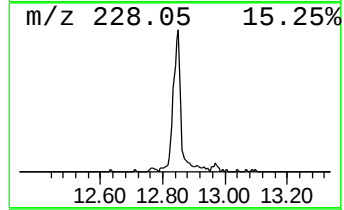
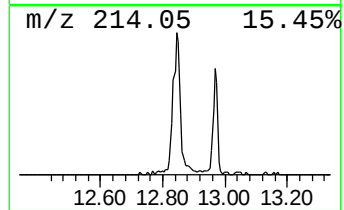
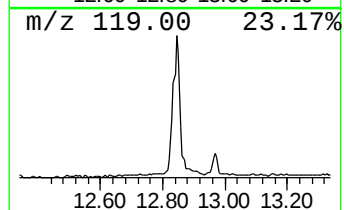
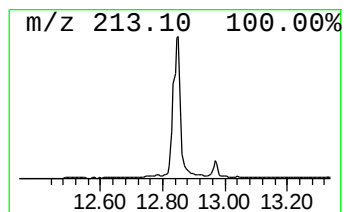
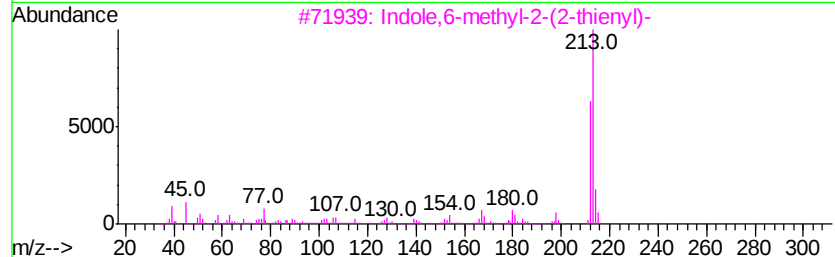
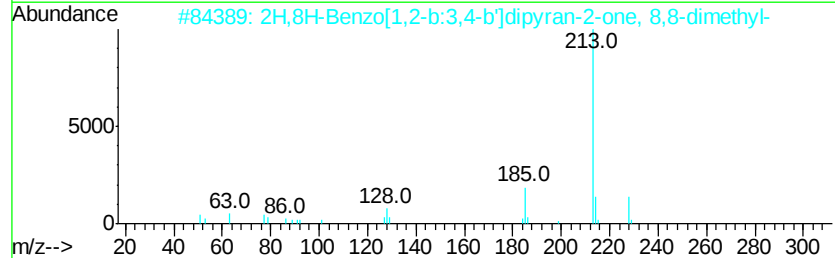
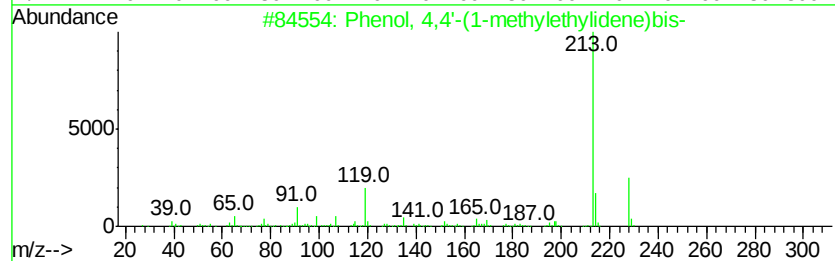
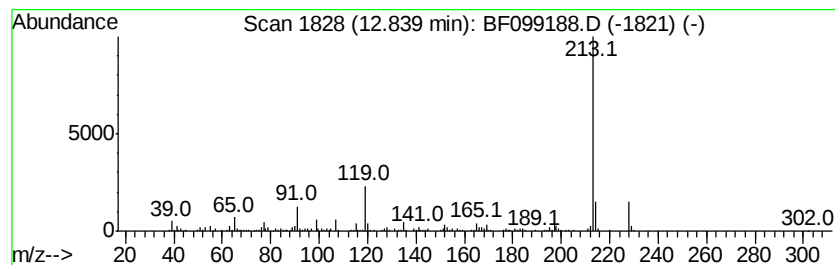
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.84	18.13 ng	630104	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97	
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53	
3	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	52	
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49	
5	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	42	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
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Sample : I5585-11
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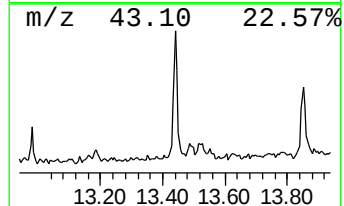
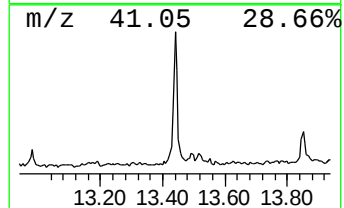
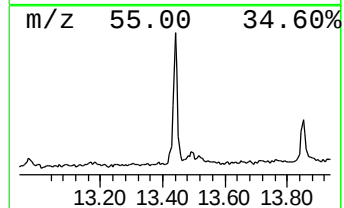
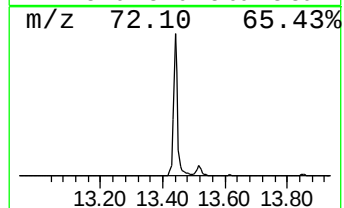
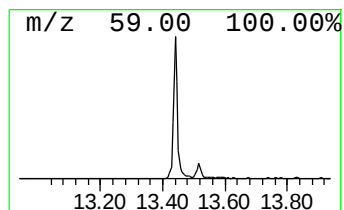
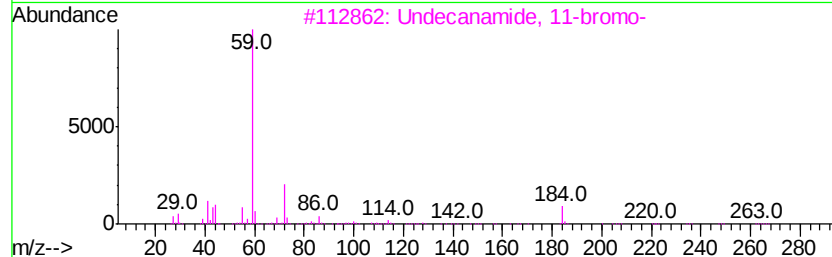
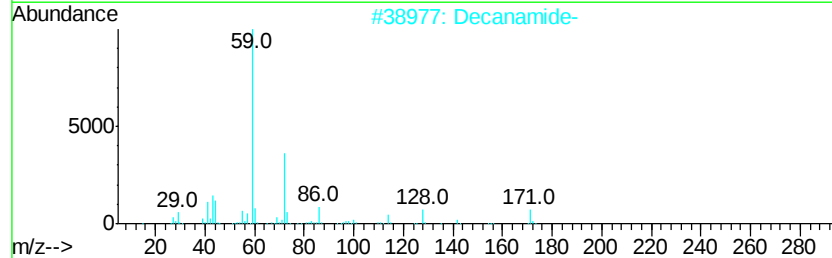
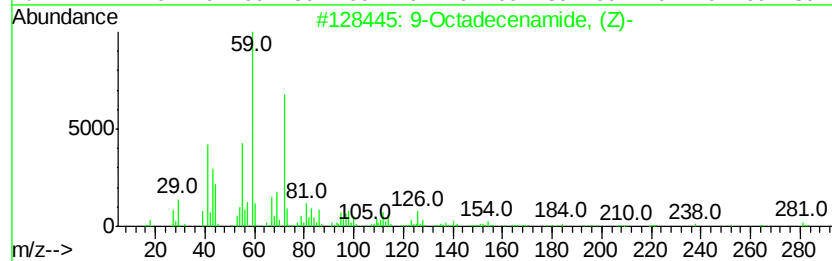
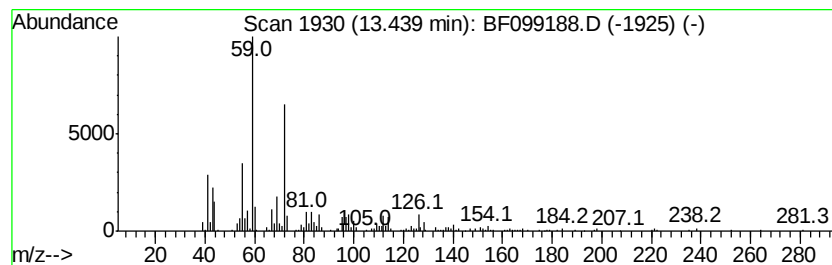
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.44	8.50 ng	295399	Chrysene-d12		14.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	Decanamide-	171	C10H21NO	002319-29-1	72
3	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	53
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
Data File : BF099188.D
Acq On : 7 Oct 2017 12:21
Operator : SJ/JU
Sample : I5585-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

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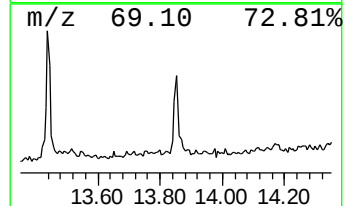
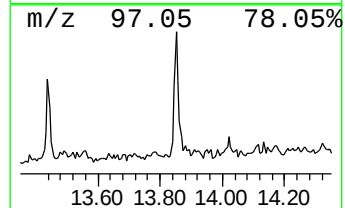
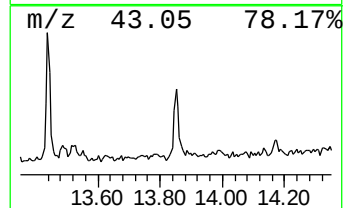
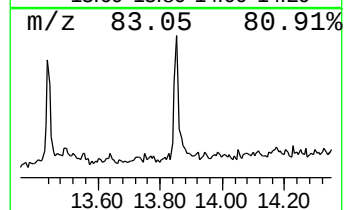
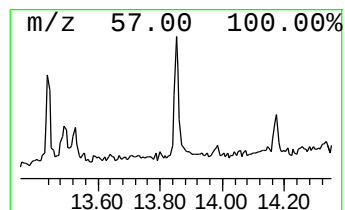
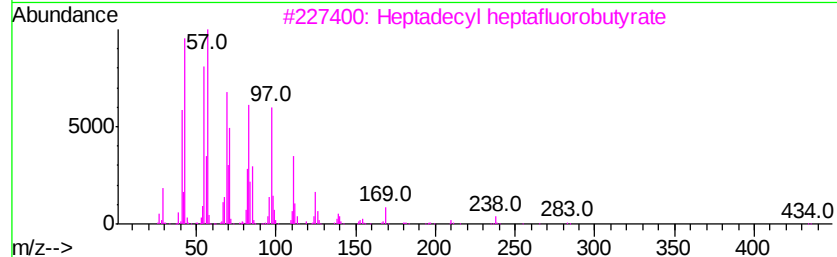
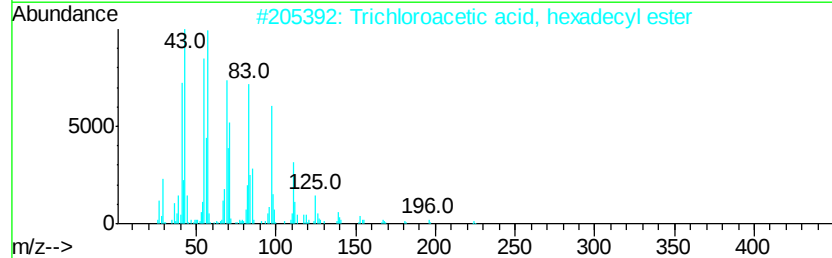
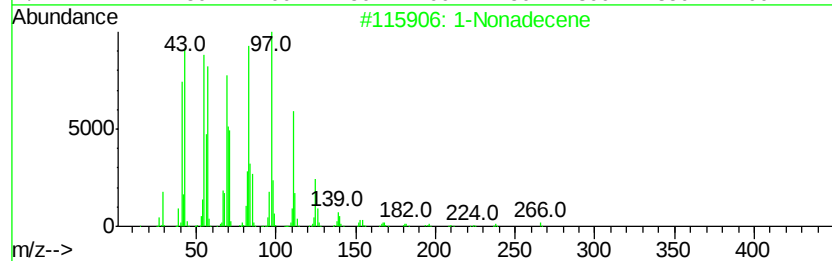
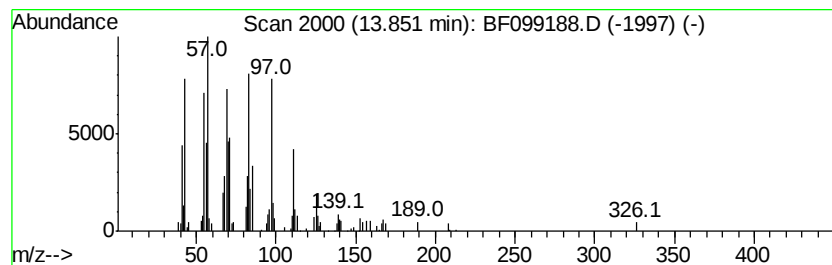
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.85 ng	99021	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	91
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Heptadecyl heptafluorobutrate	452	C21H35F7O2	959085-66-6	90
4			Cycloeicosane	280	C20H40	000296-56-0	87
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099188.D
Acq On : 7 Oct 2017 12:21
Operator : SJ/JU
Sample : I5585-11
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ALS Vial : 5 Sample Multiplier: 1

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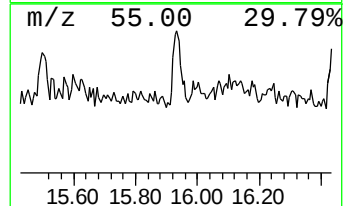
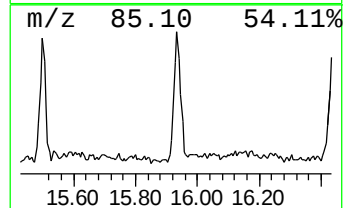
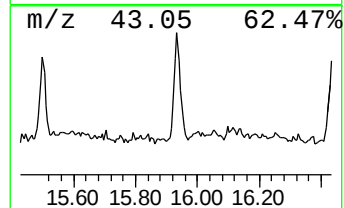
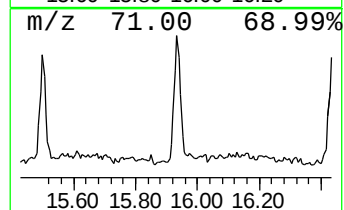
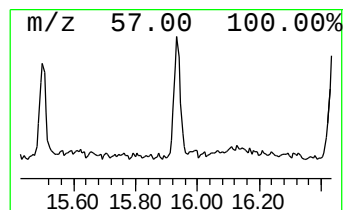
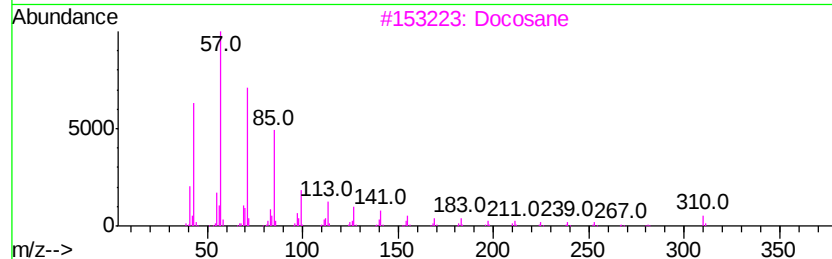
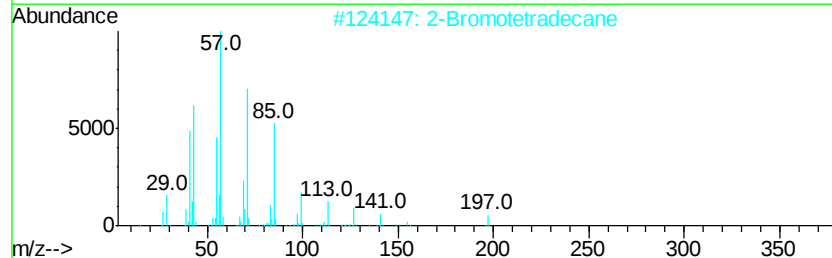
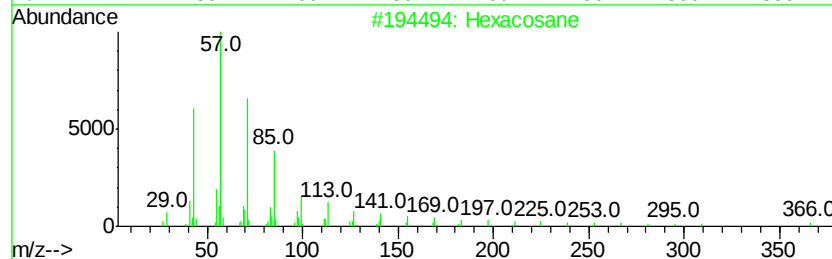
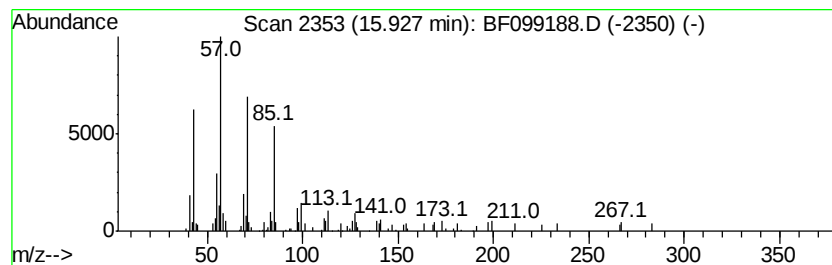
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.39 ng	92347	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		2-Bromotetradecane	276	C14H29Br	074036-95-6	86
3		Docosane	310	C22H46	000629-97-0	86
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5		Heptadecane	240	C17H36	000629-78-7	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
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Sample : I5585-11
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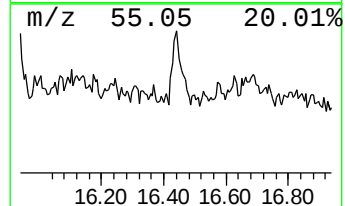
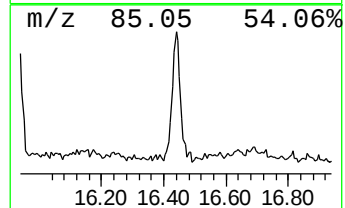
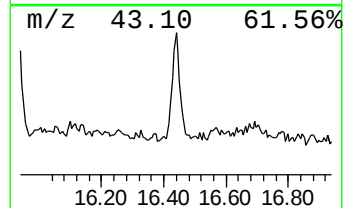
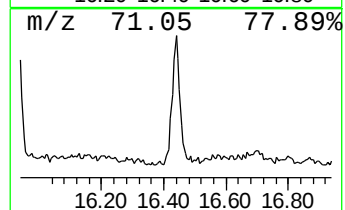
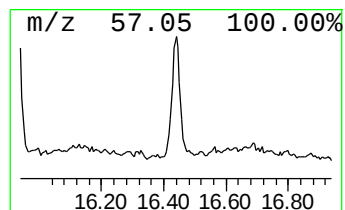
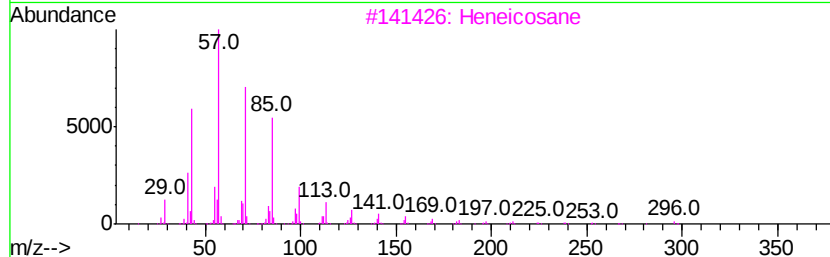
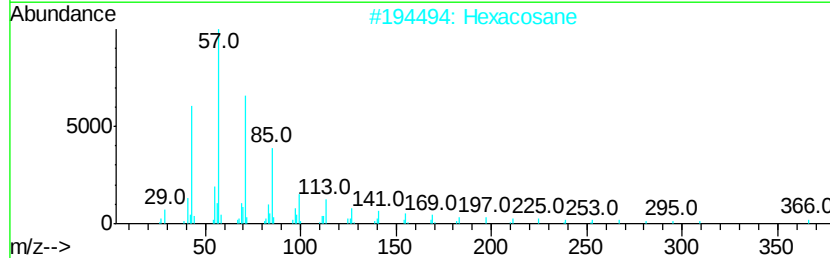
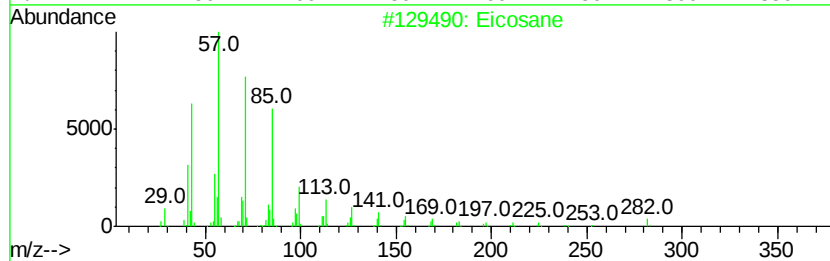
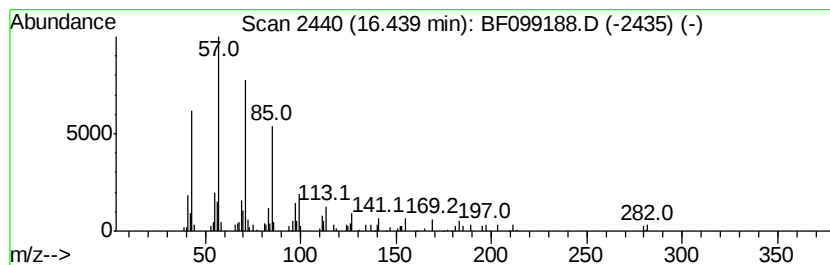
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.98 ng	115026	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282	C20H42	000112-95-8 95
2	Hexacosane	366	C26H54	000630-01-3 91
3	Heneicosane	296	C21H44	000629-94-7 91
4	Triacontane	422	C30H62	000638-68-6 91
5	Octadecane	254	C18H38	000593-45-3 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
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 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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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...	2.17	5.0	ng	195173	1	6.86	788936	20.0
3-Penten-2-one, 4...	4.47	3.0	ng	117654	1	6.86	788936	20.0
2-Pentanone, 4-hy...	5.10	15.3	ng	603376	1	6.86	788936	20.0
unknown6.64	6.64	87.2	ng	3438180	1	6.86	788936	20.0
n-Hexadecanoic acid	11.90	2.5	ng	122058	4	11.39	991450	20.0
Butyl citrate	12.77	2.1	ng	72531	5	14.02	695215	20.0
Phenol, 4,4'-(1-m...	12.84	18.1	ng	630104	5	14.02	695215	20.0
9-Octadecenamide, ...	13.44	8.5	ng	295399	5	14.02	695215	20.0
1-Nonadecene	13.85	2.9	ng	99021	5	14.02	695215	20.0
Hexacosane	15.93	2.4	ng	92347	6	15.50	771818	20.0
Eicosane	16.44	3.0	ng	115026	6	15.50	771818	20.0