

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
 Data File : BF097099.D
 Acq On : 27 Jul 2017 2:20
 Operator : SJ/JU
 Sample : I4359-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CEMETERY-4-(0-2)

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-BF072517.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	2.281	62	67	73	rVB	25934	43339	1.76%	0.215%
2	4.634	464	467	477	rBV	206810	312282	12.65%	1.551%
3	5.093	541	545	565	rBV	2248729	2428110	98.33%	12.058%
4	6.157	721	726	737	rBV	2172966	2469401	100.00%	12.263%
5	6.269	741	745	748	rBV	2444002	2244775	90.90%	11.147%
6	6.492	780	783	793	rBV	679610	612199	24.79%	3.040%
7	6.651	806	810	820	rBV	1923675	1670386	67.64%	8.295%
8	6.922	851	856	862	rBV	79650	78475	3.18%	0.390%
9	7.063	876	880	883	rBV	1473815	1339546	54.25%	6.652%
10	7.704	985	989	998	rBV	28267	33488	1.36%	0.166%
11	7.781	998	1002	1006	rBV	892560	798881	32.35%	3.967%
12	8.857	1181	1185	1188	rBV	2321052	2123138	85.98%	10.543%
13	9.257	1249	1253	1256	rBV	220535	185600	7.52%	0.922%
14	9.522	1294	1298	1302	rBV	764536	679094	27.50%	3.372%
15	9.980	1373	1376	1379	rVB	56350	42493	1.72%	0.211%
16	10.310	1428	1432	1449	rVB	1148568	1041949	42.19%	5.174%
17	10.451	1452	1456	1462	rBV	68804	80612	3.26%	0.400%
18	10.898	1527	1532	1534	rVB	26992	24876	1.01%	0.124%
19	10.998	1545	1549	1553	rVB	642245	546610	22.14%	2.714%
20	11.551	1640	1643	1647	rBV	47148	51306	2.08%	0.255%
21	12.586	1814	1819	1822	rBV	1469873	1486163	60.18%	7.380%
22	13.498	1970	1974	1981	rBV2	94562	123797	5.01%	0.615%
23	13.621	1991	1995	1999	rBV	613755	565729	22.91%	2.809%
24	14.710	2177	2180	2183	rVB2	30602	31198	1.26%	0.155%
25	14.974	2221	2225	2229	rBV	389059	402128	16.28%	1.997%
26	15.027	2231	2234	2241	rVB	61973	69648	2.82%	0.346%
27	15.168	2254	2258	2262	rBV7	23686	53588	2.17%	0.266%
28	15.386	2291	2295	2299	rBV	75709	103998	4.21%	0.516%
29	15.580	2325	2328	2333	rBV6	27427	54950	2.23%	0.273%
30	15.804	2361	2366	2373	rVB2	81063	147445	5.97%	0.732%
31	16.280	2443	2447	2453	rVB3	55119	99650	4.04%	0.495%
32	16.498	2483	2484	2490	rBV6	17052	32656	1.32%	0.162%
33	16.851	2537	2544	2553	rVB3	58846	160051	6.48%	0.795%

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ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
CEMETERY-4-(0-2)

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-BF072517.M
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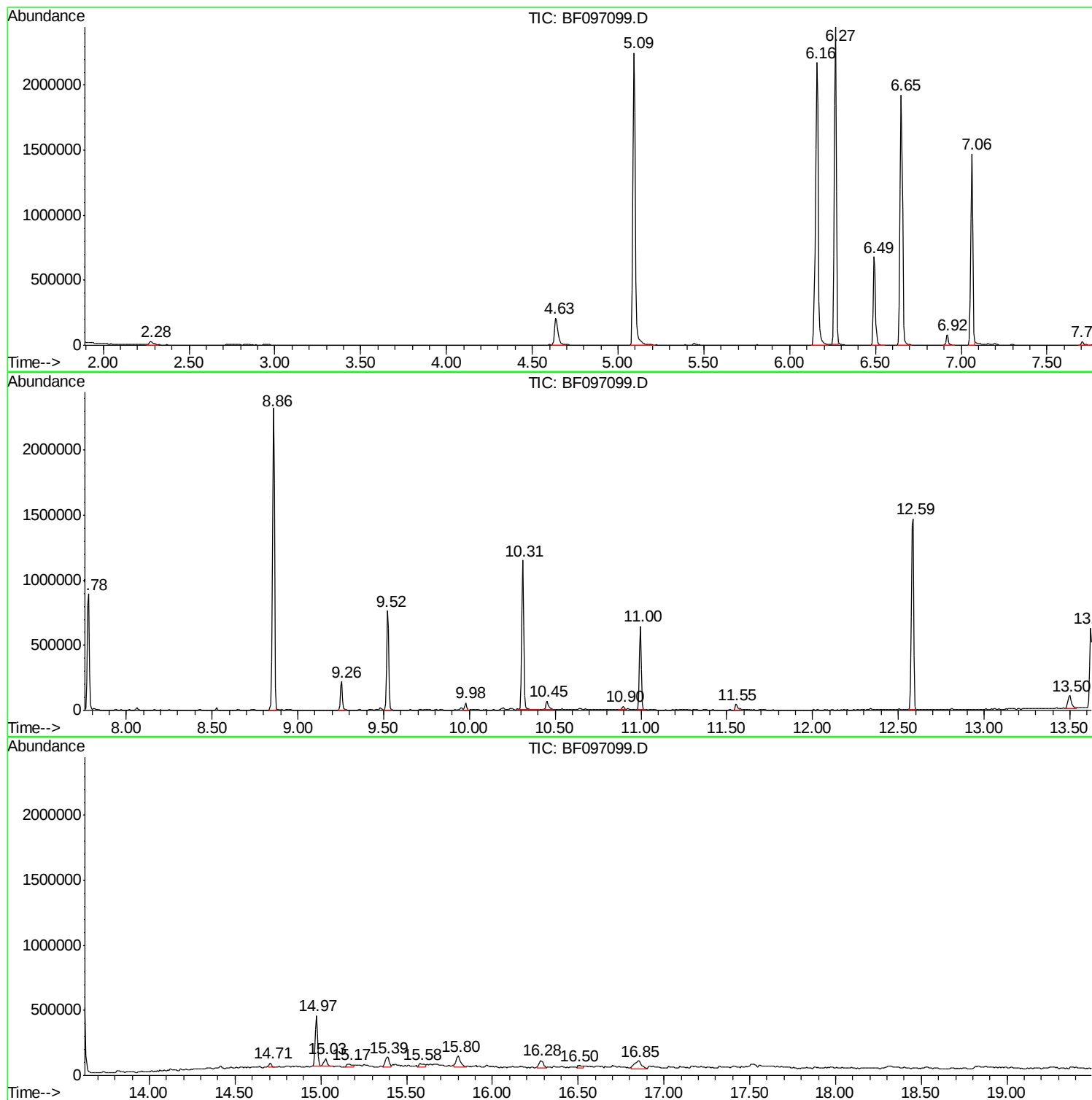
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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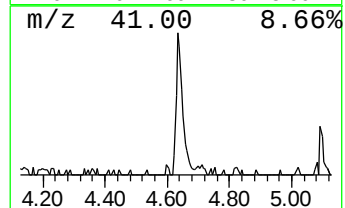
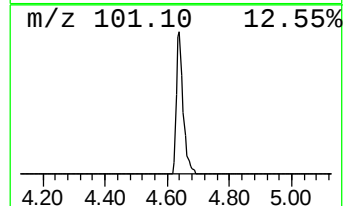
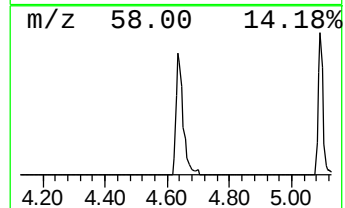
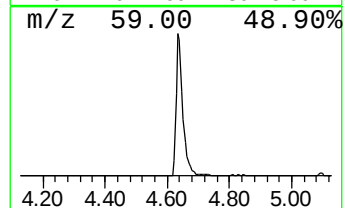
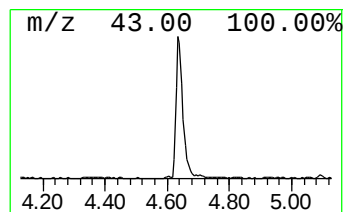
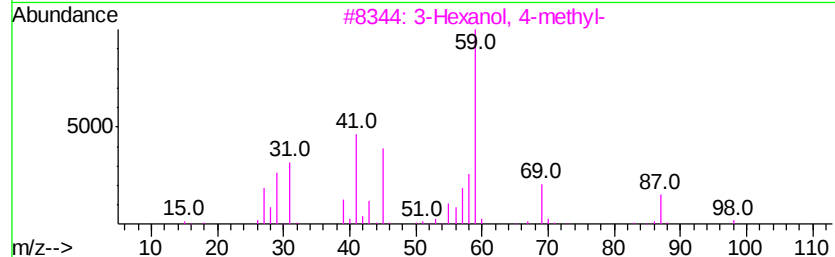
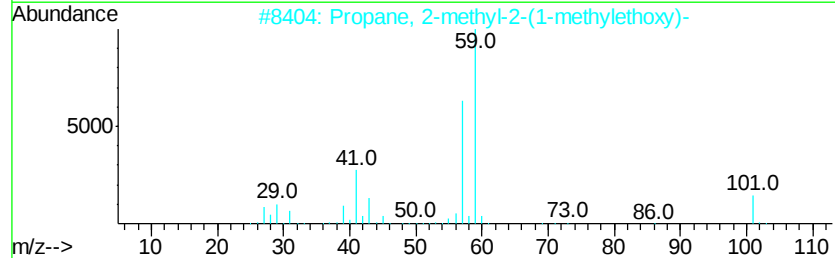
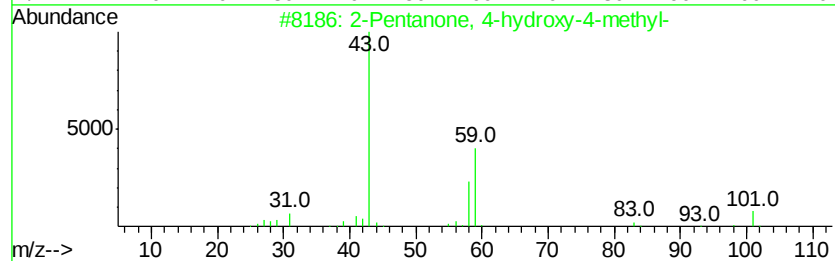
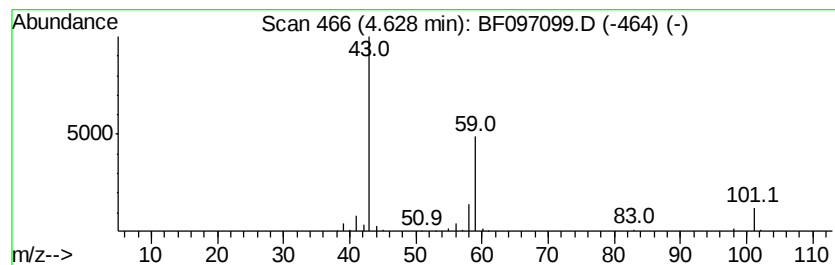
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	10.20 ng	312282	1,4-Dichlorobenzene-d4	6.49

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-methylethoxy)-	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5		4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	17



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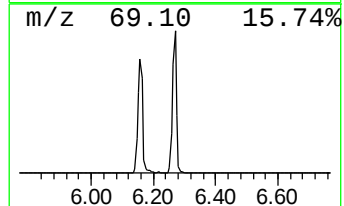
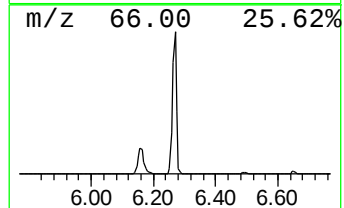
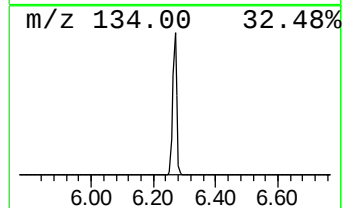
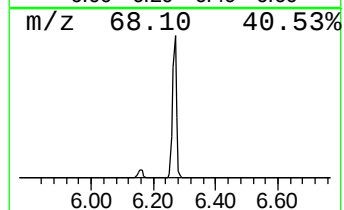
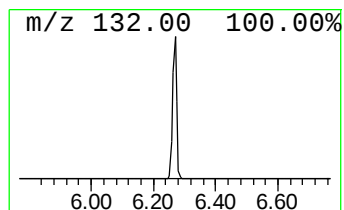
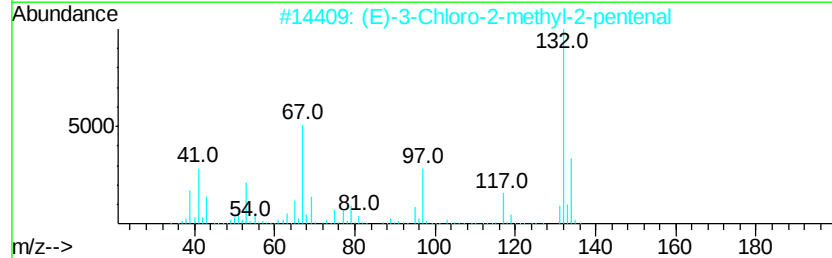
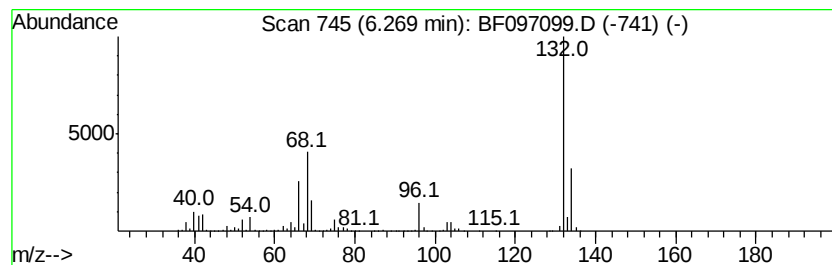
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	73.33 ng	2244780	1,4-Dichlorobenzene-d4	6.49

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicvano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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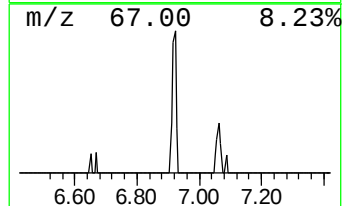
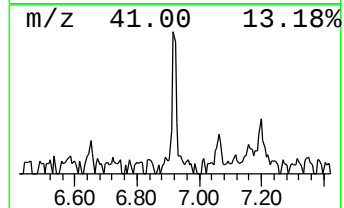
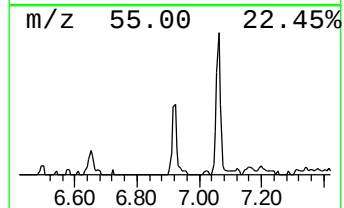
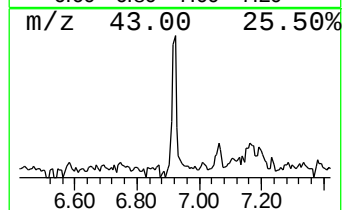
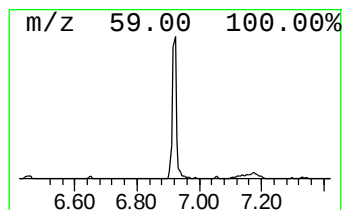
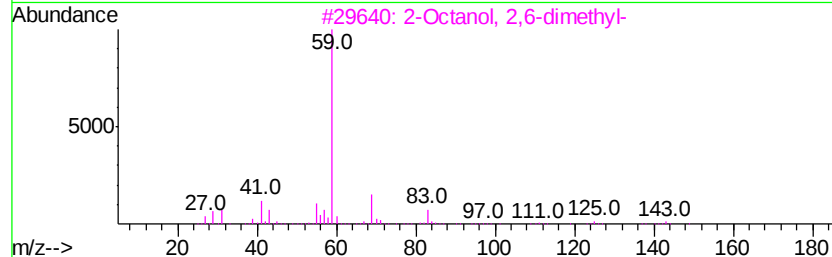
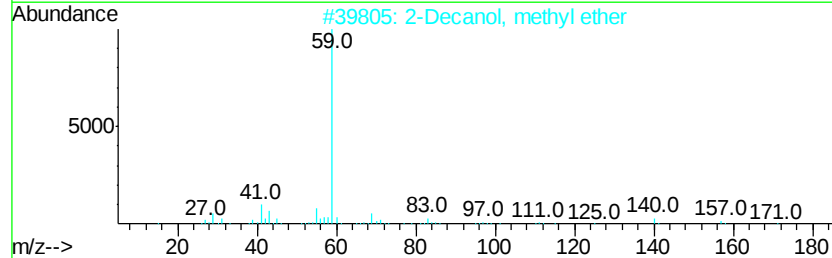
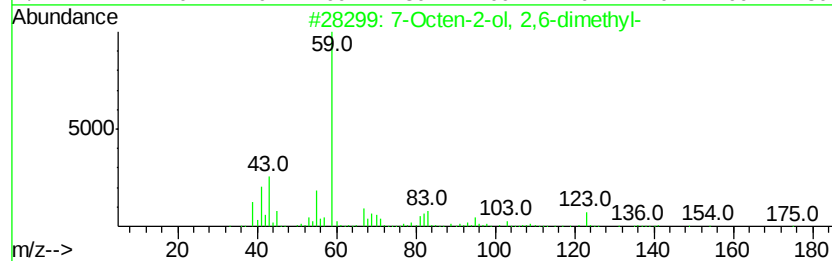
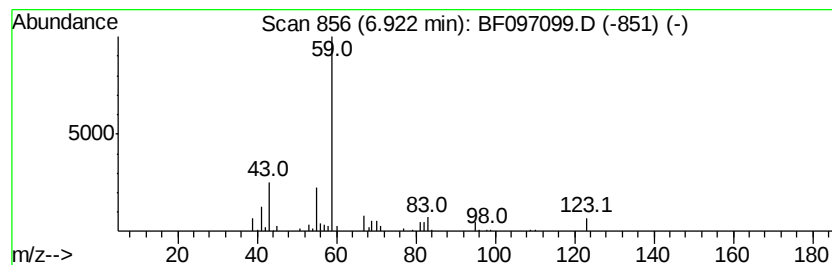
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	2.56 ng	78475	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2		2-Decanol, methyl ether	172	C11H24O	1000333-83-9	59
3		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	50
5		1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	43



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ALS Vial : 20 Sample Multiplier: 1

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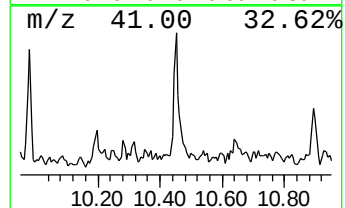
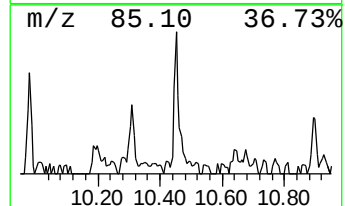
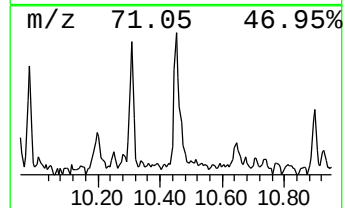
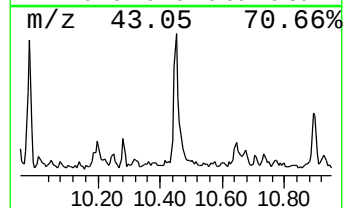
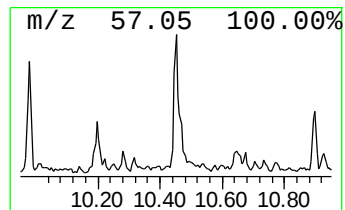
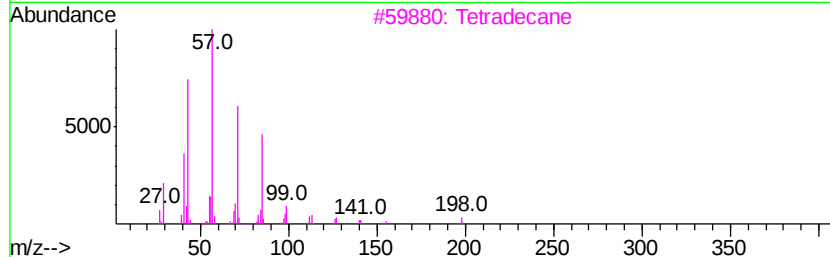
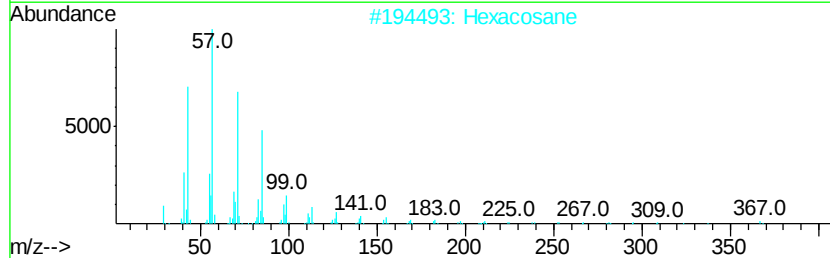
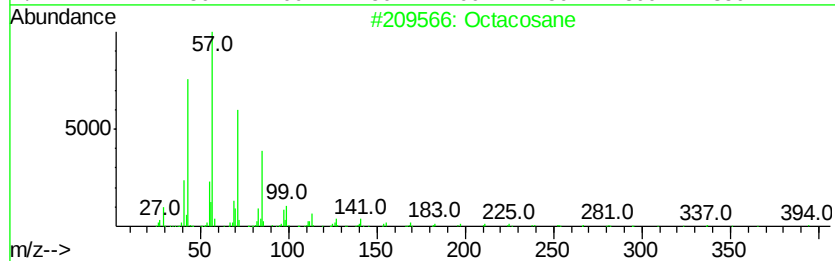
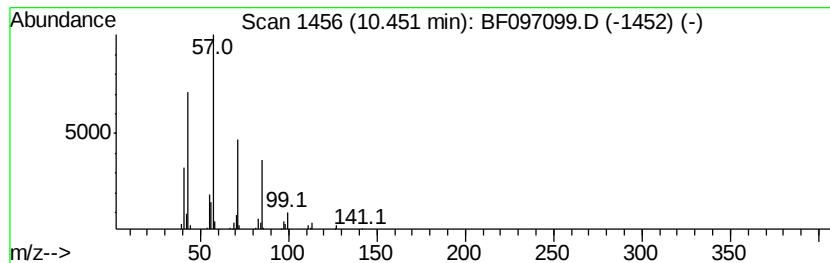
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.95 ng	80612	Phenanthrene-d10	11.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hexacosane		366	C26H54	000630-01-3	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Tridecane		184	C13H28	000629-50-5	86
5	Hexadecane		226	C16H34	000544-76-3	86



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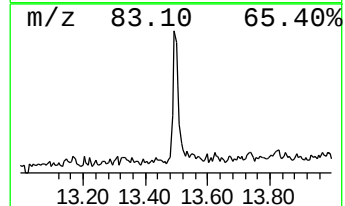
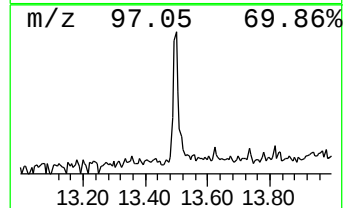
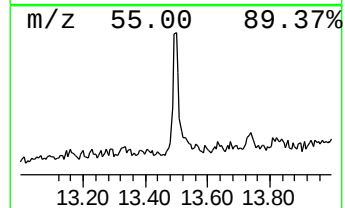
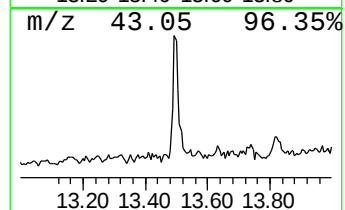
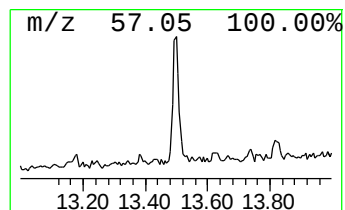
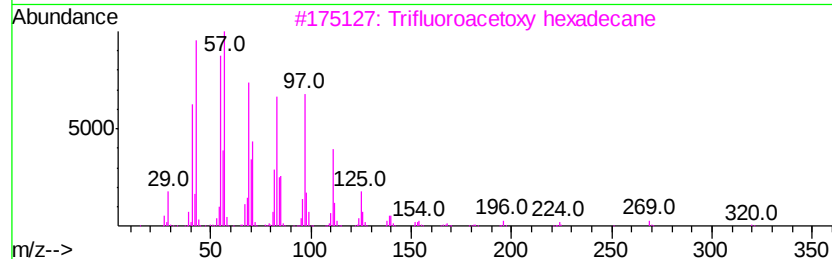
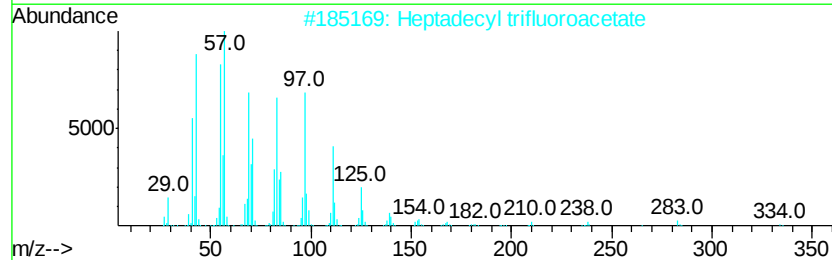
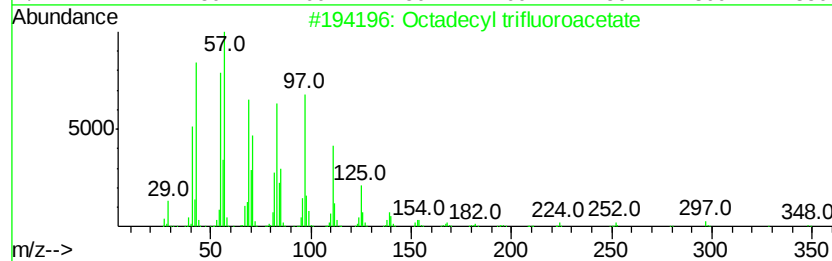
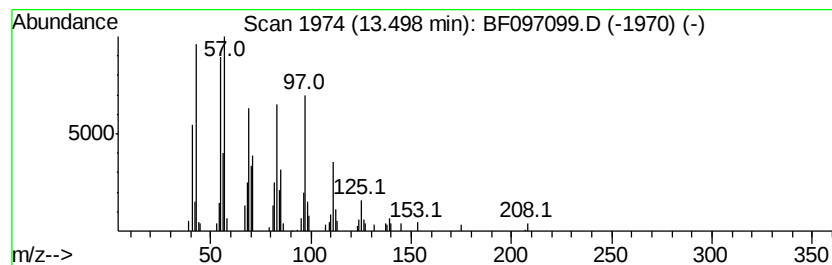
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	4.38 ng	123797	Chrysene-d12	13.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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CEMETERY-4-(0-2)

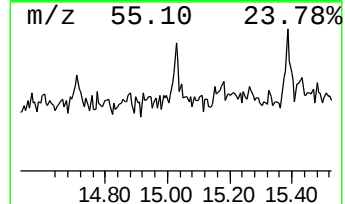
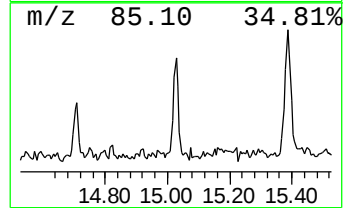
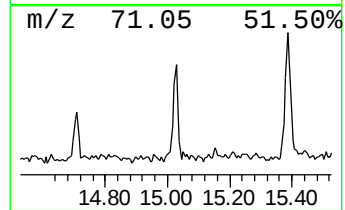
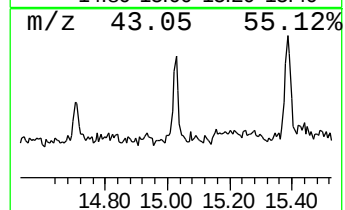
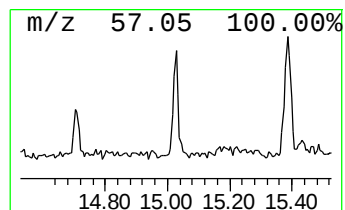
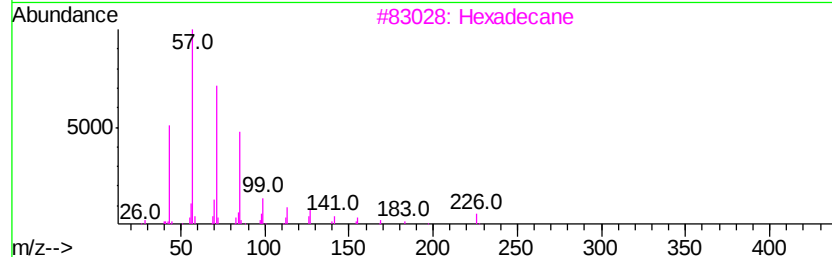
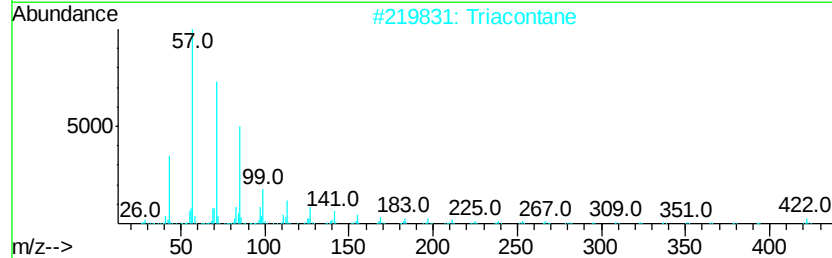
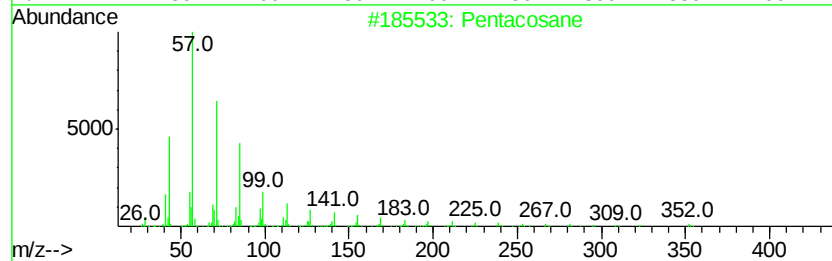
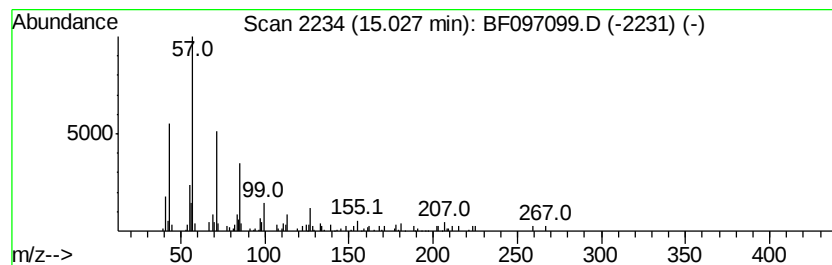
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	3.46 ng	69648	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	83
2		Triacontane	422	C30H62	000638-68-6	80
3		Hexadecane	226	C16H34	000544-76-3	80
4		Hexacosane	366	C26H54	000630-01-3	74
5		Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
Sample : I4359-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CEMETERY-4-(0-2)

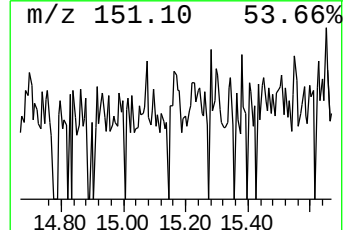
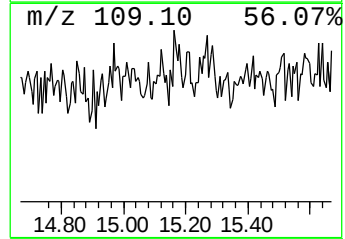
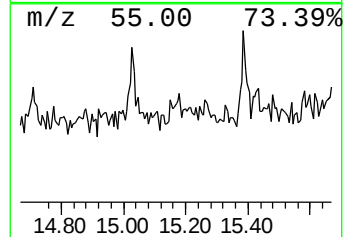
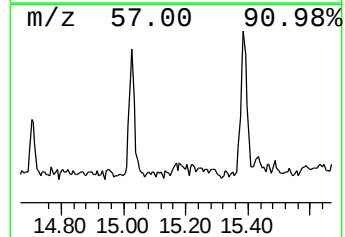
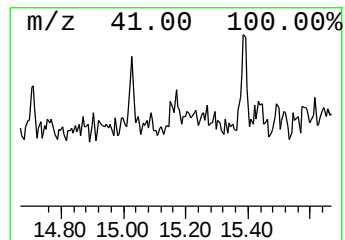
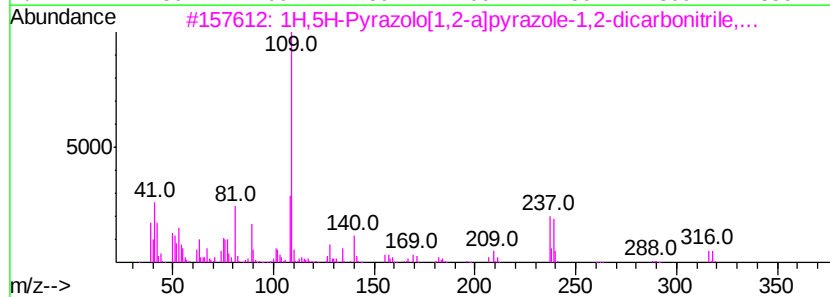
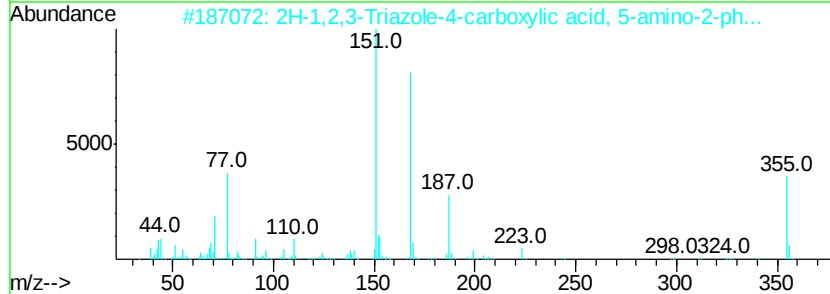
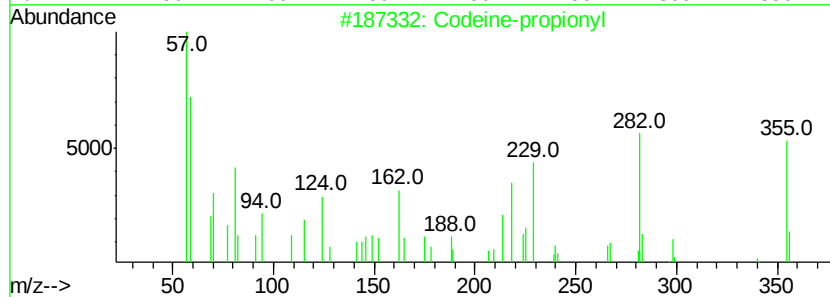
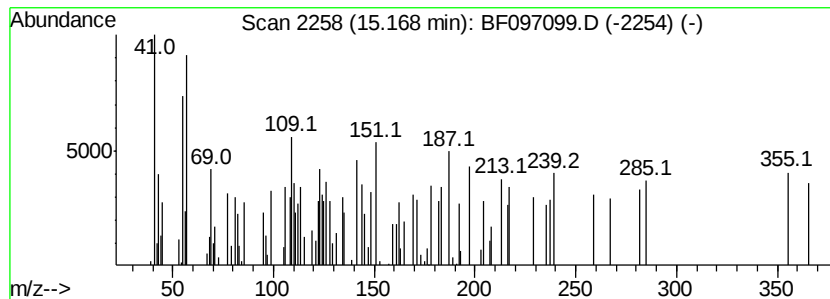
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.17 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.67 ng	53588	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Codeine-propionyl	355	C21H25NO4	065644-90-8	10
2		2H-1,2,3-Triazole-4-carboxylic a...	355	C15H17N9O2	1000316-28-9	7
3		1H,5H-Pyrazolo[1,2-a]pyrazole-1,...	316	C14H13BrN4	1000319-94-2	1



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
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ClientSampleId :
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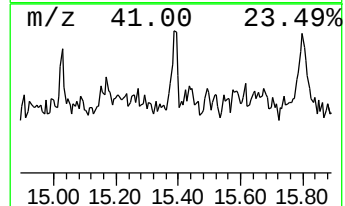
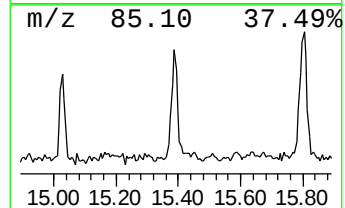
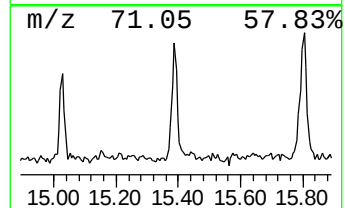
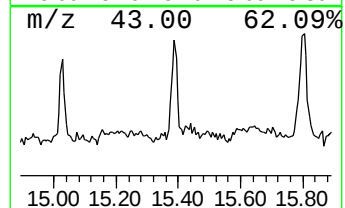
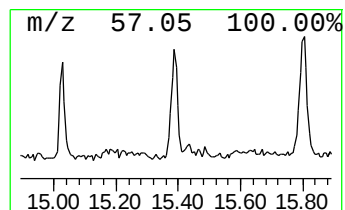
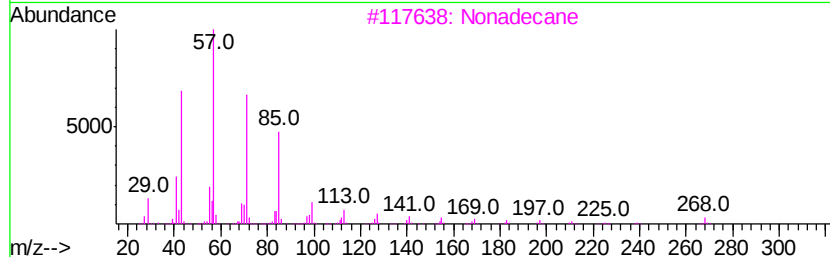
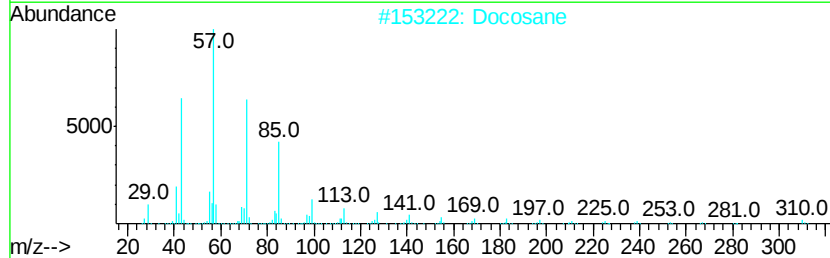
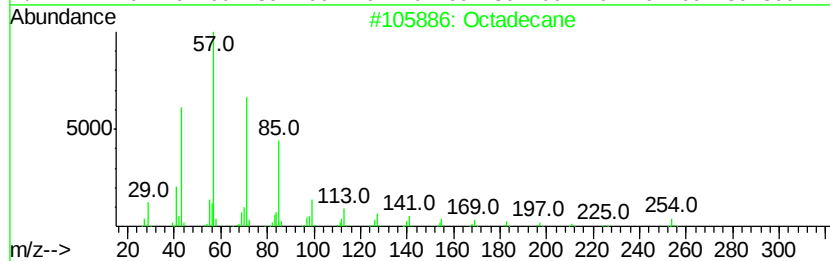
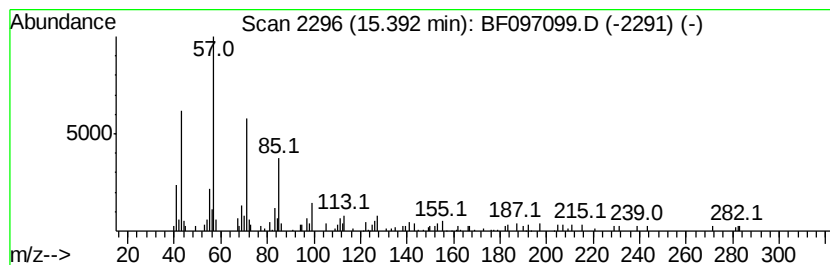
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	5.17 ng	103998	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Docosane	310	C22H46	000629-97-0	90
3		Nonadecane	268	C19H40	000629-92-5	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
Sample : I4359-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CEMETERY-4-(0-2)

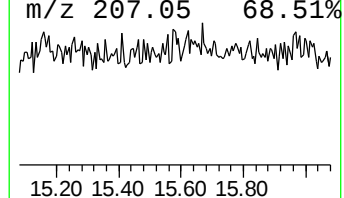
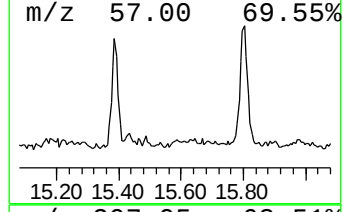
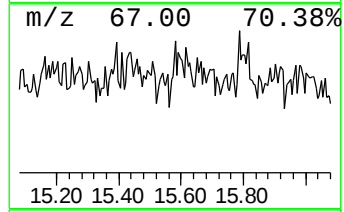
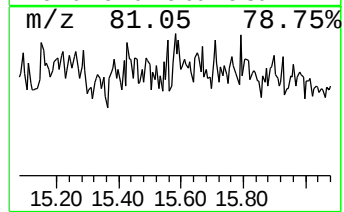
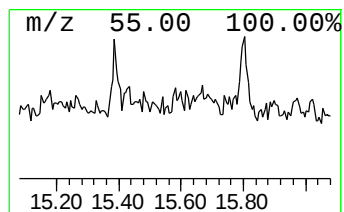
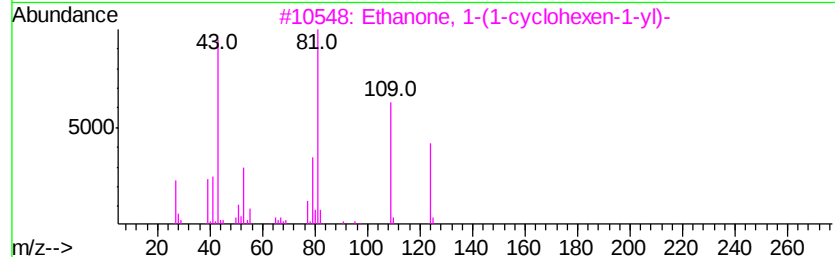
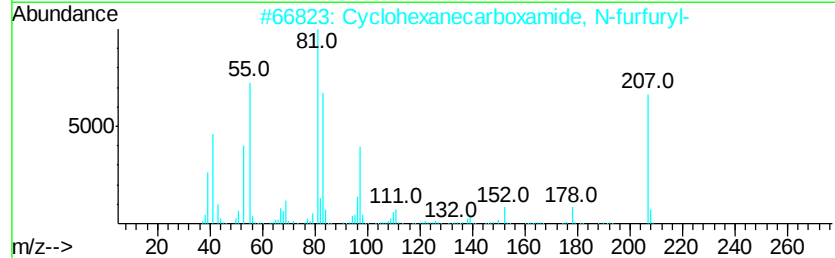
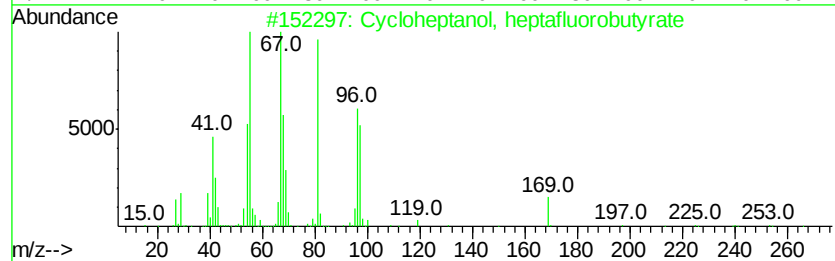
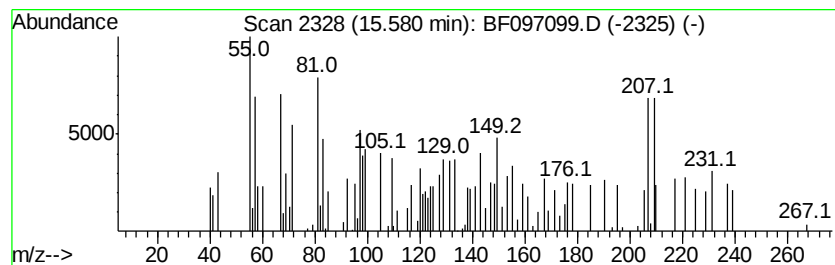
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.58 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.73 ng	54950	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptanol, heptafluorobutyrate	310	C11H13F7O2	1000376-25-6	14
2			Cyclohexanecarboxamide, N-furfuryl-	207	C12H17NO2	006341-32-8	12
3			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	10
4			dl-.beta.-Ethyl-3-dimethylamino-...	203	C10H21NO3	1000298-96-2	10
5			6-Nonenal, 3,7-dimethyl-	168	C11H20O	1000132-43-9	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
CEMETERY-4-(0-2)

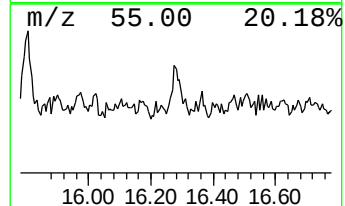
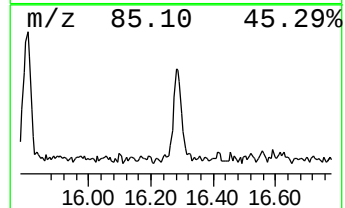
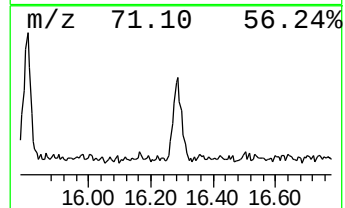
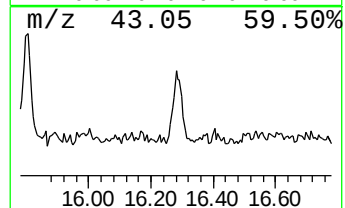
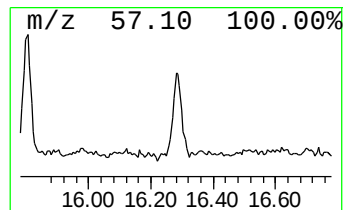
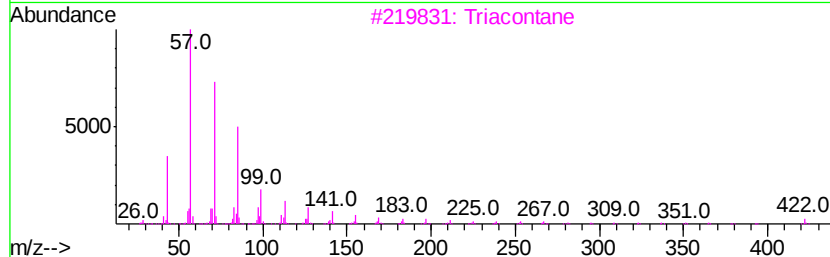
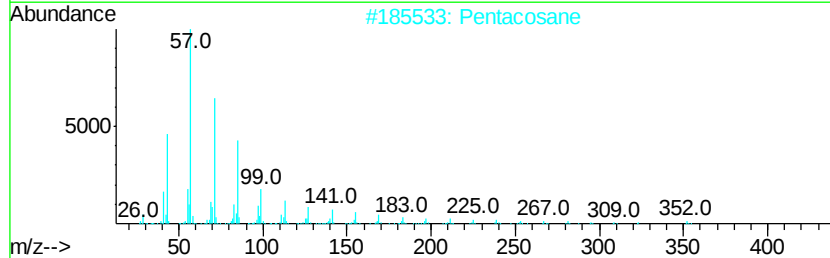
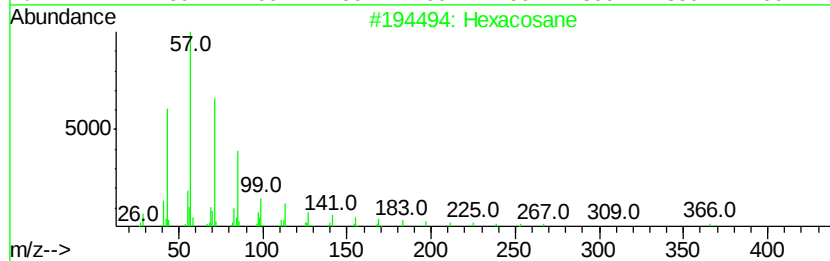
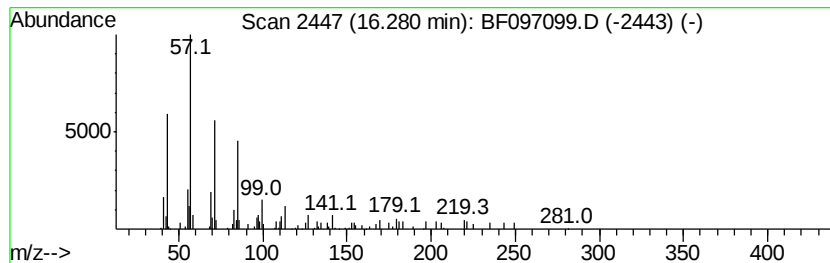
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	4.96 ng	99650	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Pentacosane	352	C25H52	000629-99-2	83
3			Triacontane	422	C30H62	000638-68-6	83
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5			Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
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Misc :
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ClientSampleId :
CEMETERY-4-(0-2)

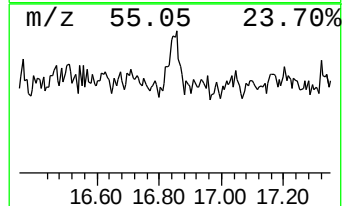
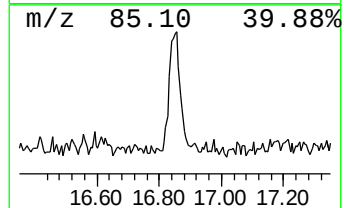
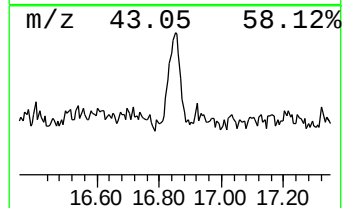
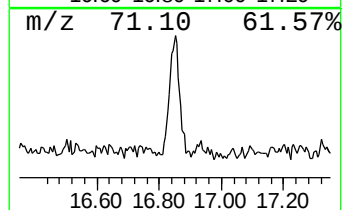
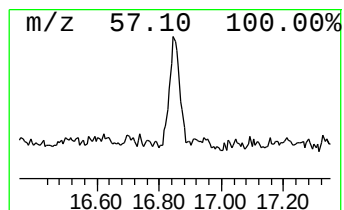
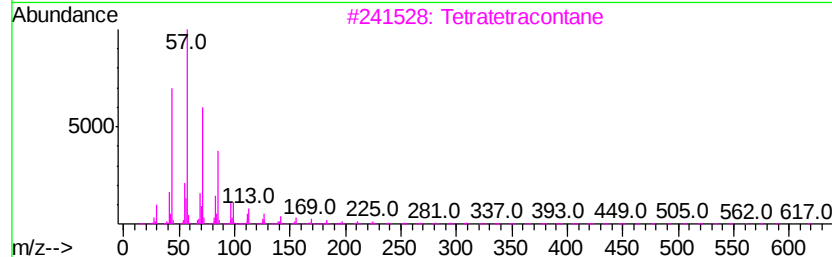
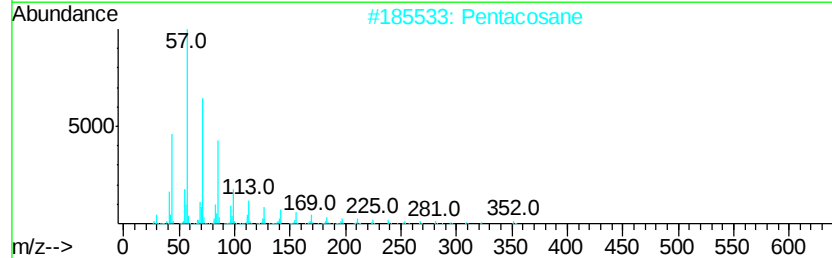
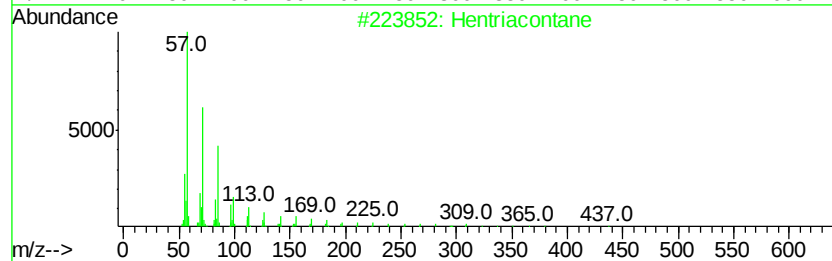
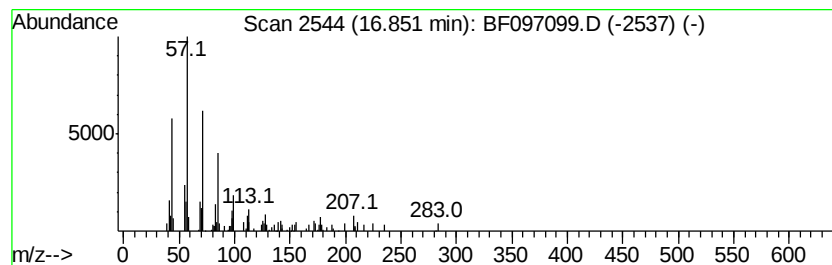
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.85	7.96 ng	160051	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Pentacosane	352	C25H52	000629-99-2	83
3		Tetratetracontane	619	C44H90	007098-22-8	83
4		Hexacosane	366	C26H54	000630-01-3	83
5		2-methyloctacosane	408	C29H60	1000376-72-8	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097099.D
Acq On : 27 Jul 2017 2:20
Operator : SJ/JU
Sample : I4359-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.27	6.27	73.3	ng	2244780	1	6.49	612199	20.0
7-Octen-2-ol, 2,6...	6.92	2.6	ng	78475	1	6.49	612199	20.0
Octacosane	10.45	3.0	ng	80612	4	11.00	546610	20.0
Octadecyl trifluo...	13.50	4.4	ng	123797	5	13.62	565729	20.0
Pentacosane	15.03	3.5	ng	69648	6	14.97	402128	20.0
unknown15.17	15.17	2.7	ng	53588	6	14.97	402128	20.0
Octadecane	15.39	5.2	ng	103998	6	14.97	402128	20.0
unknown15.58	15.58	2.7	ng	54950	6	14.97	402128	20.0
Hexacosane	16.28	5.0	ng	99650	6	14.97	402128	20.0
Hentriacontane	16.85	8.0	ng	160051	6	14.97	402128	20.0