

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
 Data File : BF097091.D
 Acq On : 26 Jul 2017 22:38
 Operator : SJ/JU
 Sample : I4360-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 295-N-5-(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	2.310	65	72	80	rBV	110474	174069	6.09%	0.698%
2	4.645	466	469	487	rBV	219099	368811	12.91%	1.480%
3	5.098	542	546	560	rBV	2448224	2746824	96.14%	11.021%
4	6.157	721	726	738	rBV	2379630	2857135	100.00%	11.463%
5	6.269	741	745	748	rBV	2809269	2641231	92.44%	10.597%
6	6.492	780	783	793	rBV	752416	666134	23.31%	2.673%
7	6.651	806	810	813	rBV	2152544	1934668	67.71%	7.762%
8	7.063	875	880	883	rBV	1810584	1783599	62.43%	7.156%
9	7.775	997	1001	1006	rBV	980754	893927	31.29%	3.587%
10	8.857	1180	1185	1188	rBV	2674196	2628470	92.00%	10.546%
11	9.257	1249	1253	1256	rBV	310297	270518	9.47%	1.085%
12	9.480	1283	1291	1294	rBV2	30119	31028	1.09%	0.124%
13	9.521	1294	1298	1302	rBV2	1069922	974985	34.12%	3.912%
14	9.980	1373	1376	1379	rVB	65363	52115	1.82%	0.209%
15	10.198	1407	1413	1415	rBV	34501	43278	1.51%	0.174%
16	10.310	1428	1432	1439	rBV	1647715	1610016	56.35%	6.460%
17	10.451	1452	1456	1464	rBV	106693	131173	4.59%	0.526%
18	10.892	1528	1531	1534	rBV	41303	37889	1.33%	0.152%
19	10.998	1545	1549	1553	rBV	951293	799161	27.97%	3.206%
20	11.551	1641	1643	1646	rBV2	59255	52201	1.83%	0.209%
21	12.586	1814	1819	1822	rBV	2225331	2233602	78.18%	8.962%
22	13.492	1970	1973	1979	rBV	160468	189985	6.65%	0.762%
23	13.621	1991	1995	2002	rVB	677172	629168	22.02%	2.524%
24	14.127	2077	2081	2085	rBV2	37497	47466	1.66%	0.190%
25	14.704	2176	2179	2189	rBV	62613	87036	3.05%	0.349%
26	14.968	2220	2224	2230	rBV	437855	512660	17.94%	2.057%
27	15.386	2291	2295	2298	rBV2	50979	68713	2.40%	0.276%
28	15.427	2298	2302	2311	rVB4	24181	38447	1.35%	0.154%
29	16.033	2402	2405	2411	rVB6	23153	36383	1.27%	0.146%
30	16.280	2442	2447	2452	rBV2	42493	68444	2.40%	0.275%
31	16.456	2473	2477	2482	rVB4	45946	76401	2.67%	0.307%
32	16.662	2506	2512	2523	rBV4	20340	60783	2.13%	0.244%
33	16.809	2531	2537	2541	rBV7	16058	38345	1.34%	0.154%
34	17.186	2594	2601	2615	rBV2	52005	139619	4.89%	0.560%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
295-N-5-(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
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

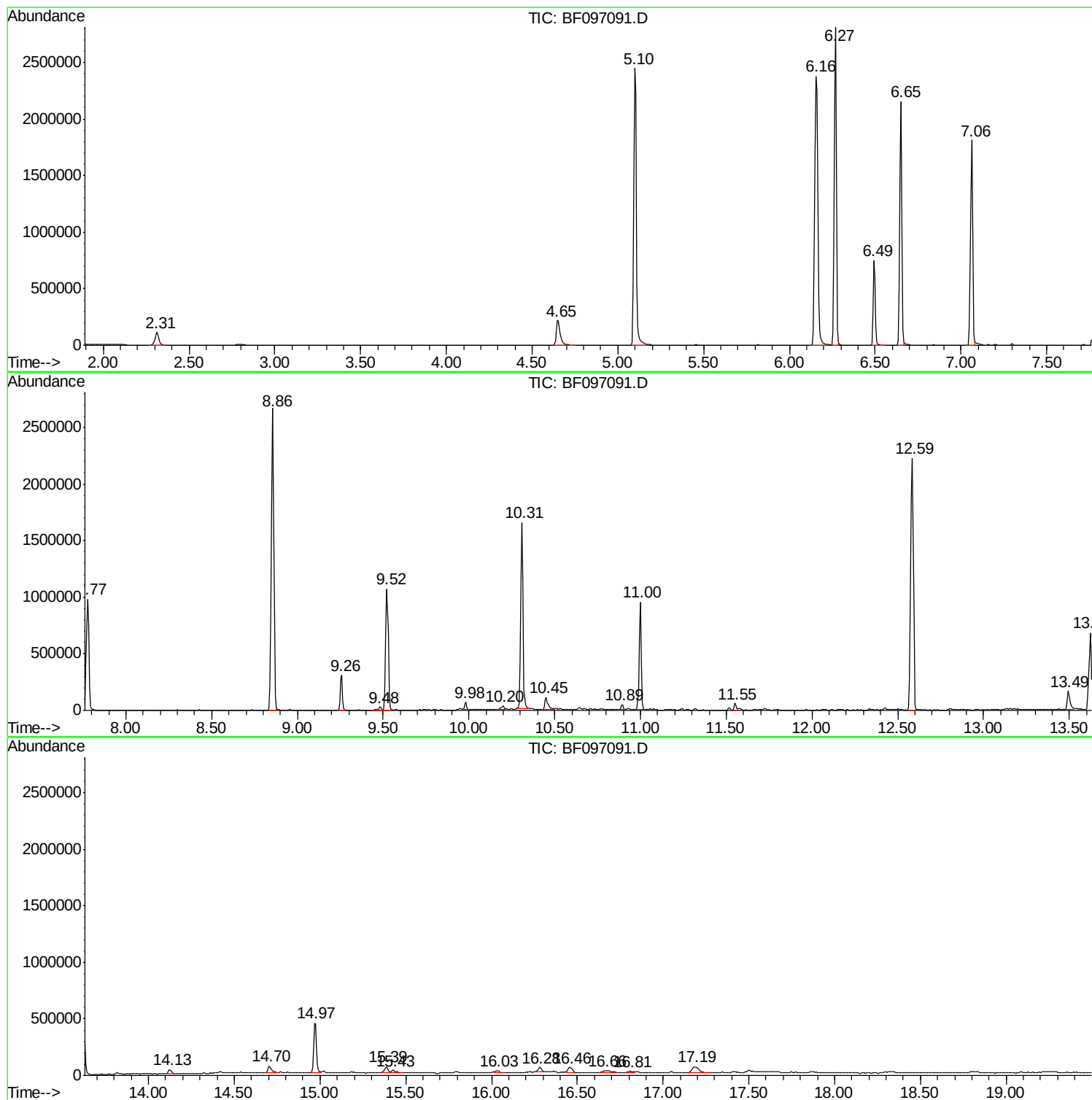
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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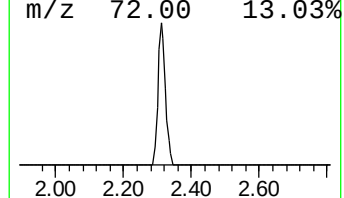
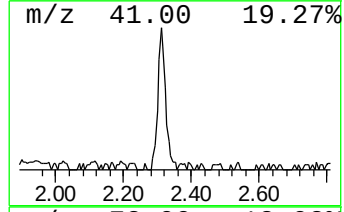
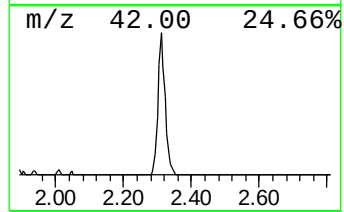
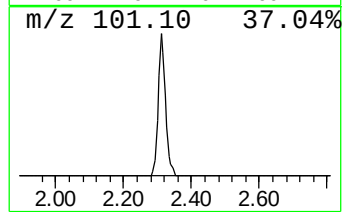
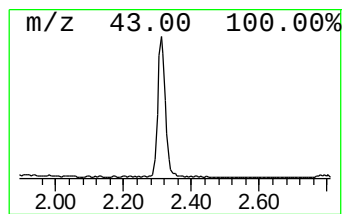
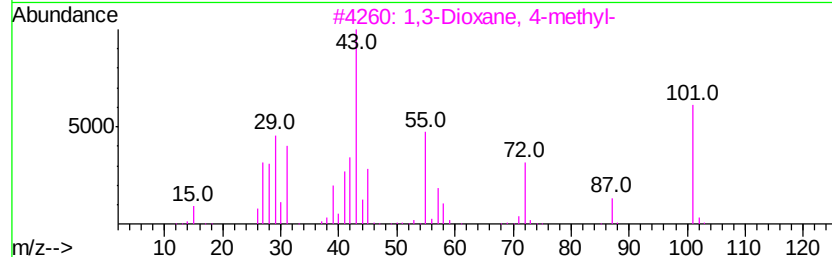
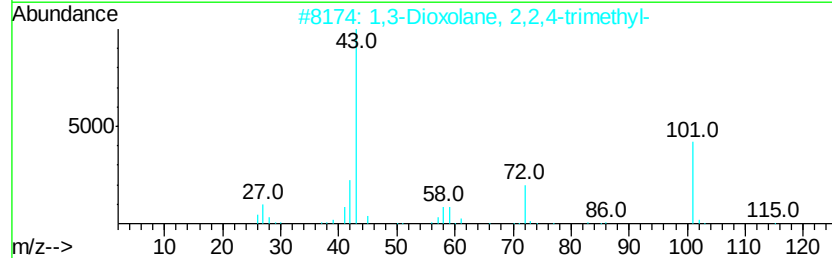
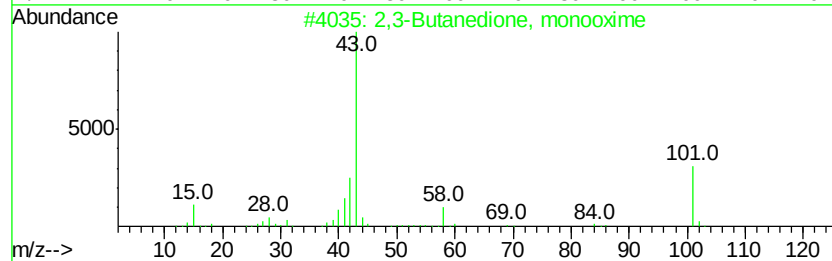
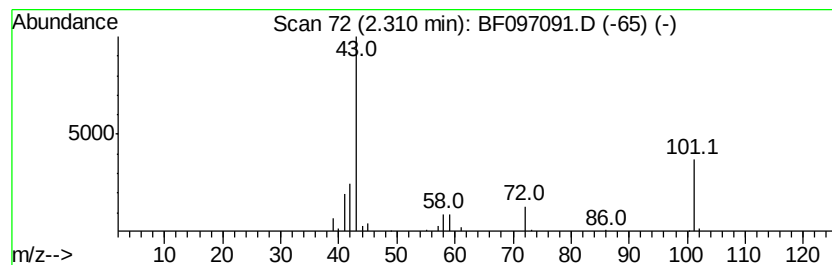
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,3-Butanedione, monooxime Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	5.23 ng	174069	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	59
2			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	59
3			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	33
4			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	33
5			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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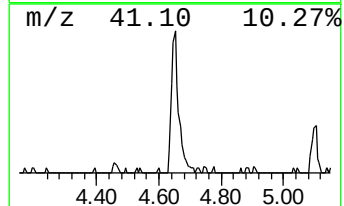
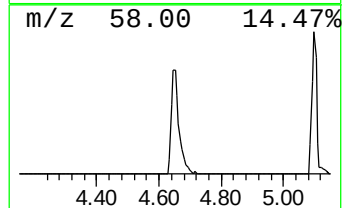
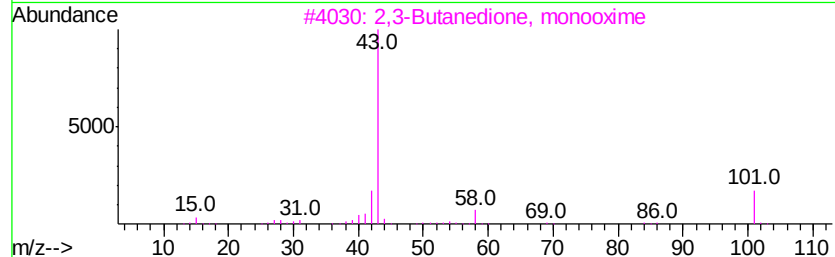
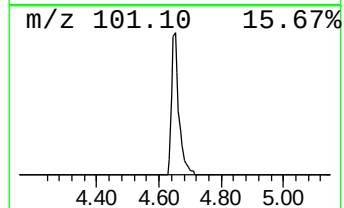
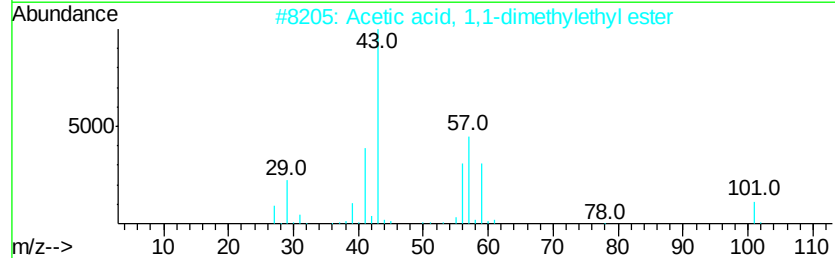
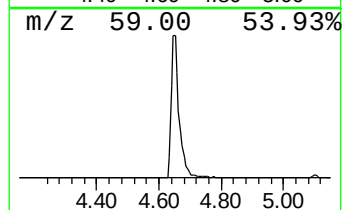
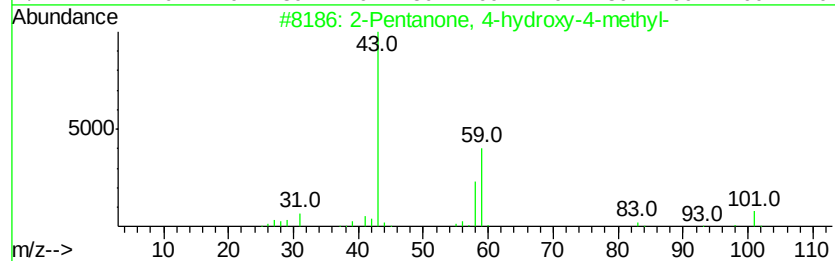
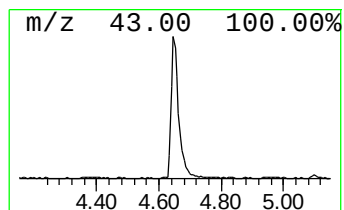
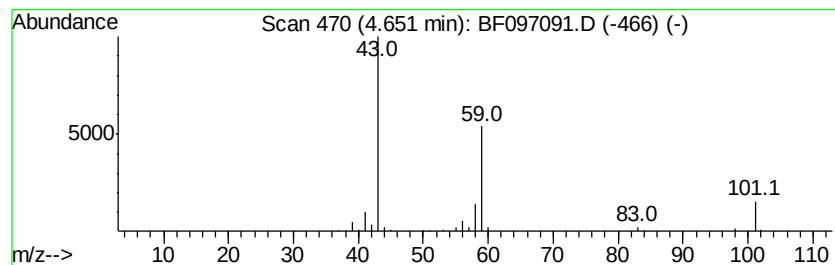
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	11.07 ng	368811	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	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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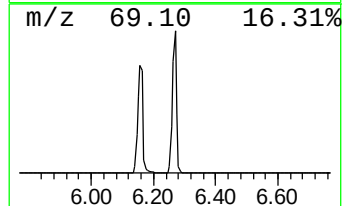
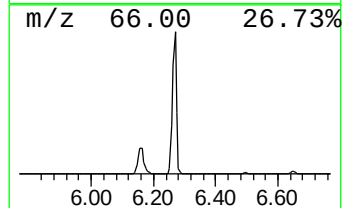
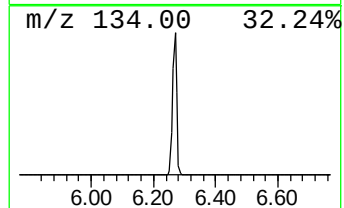
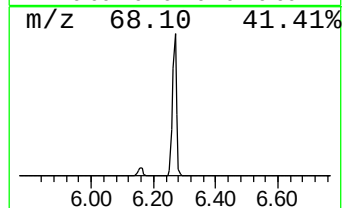
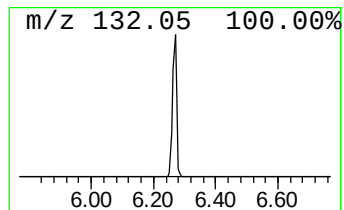
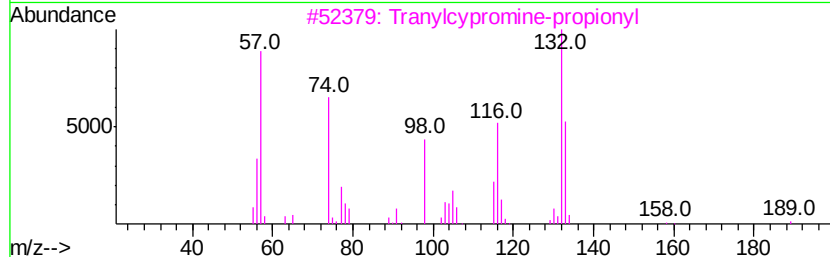
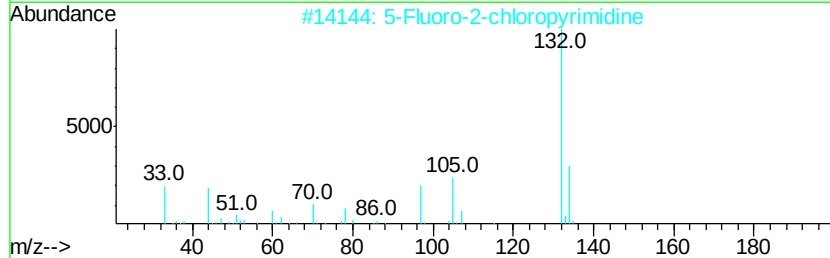
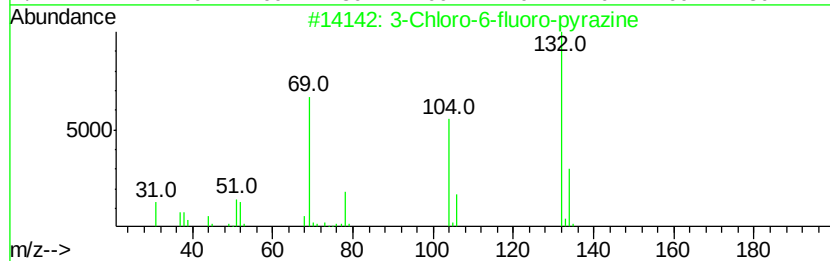
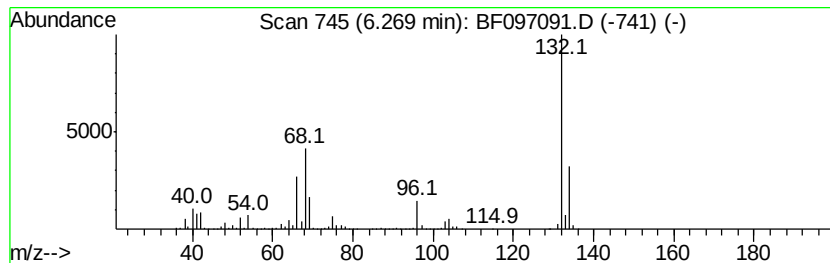
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	79.30 ng	2641230	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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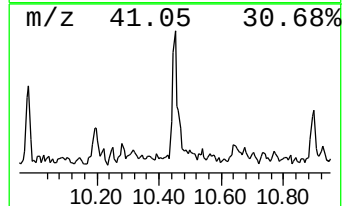
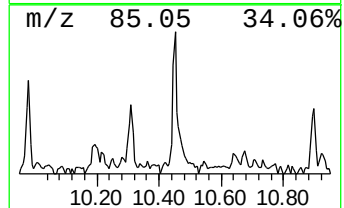
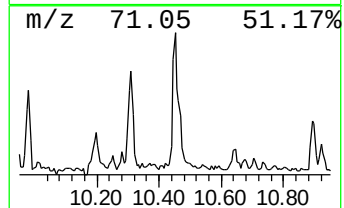
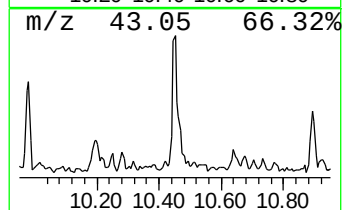
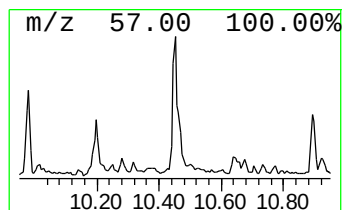
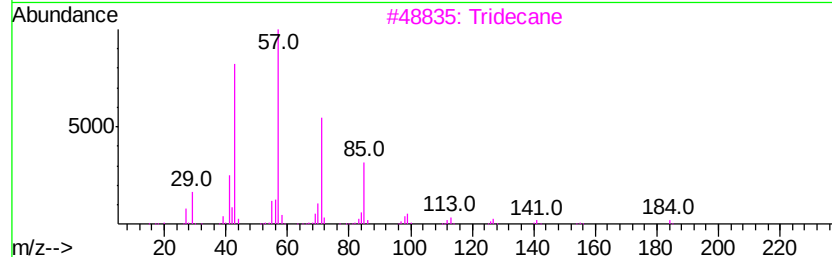
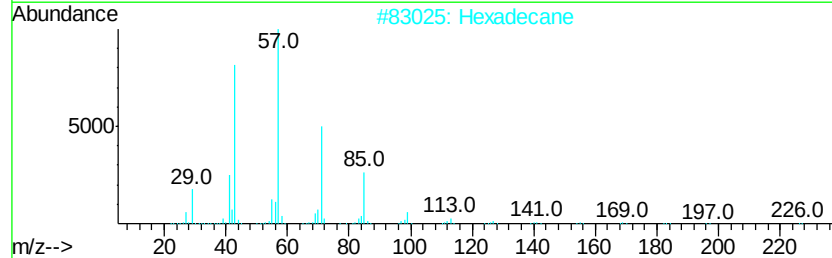
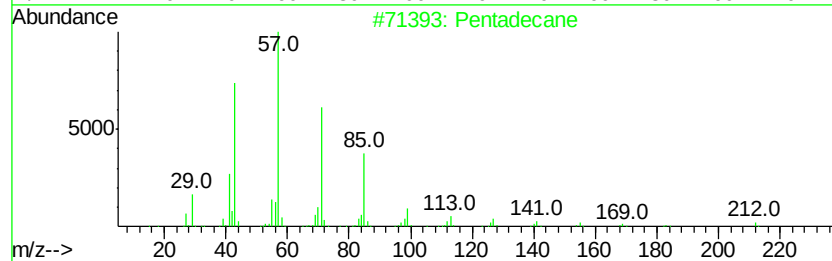
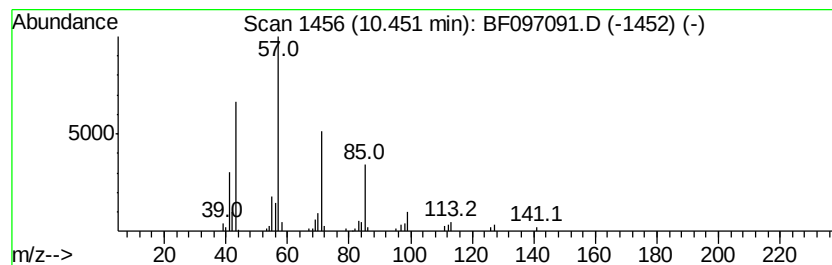
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	3.28 ng	131173	Phenanthrene-d10	11.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	90
2		Hexadecane	226	C16H34	000544-76-3	90
3		Tridecane	184	C13H28	000629-50-5	90
4		Heptadecane	240	C17H36	000629-78-7	90
5		Tetradecane	198	C14H30	000629-59-4	86



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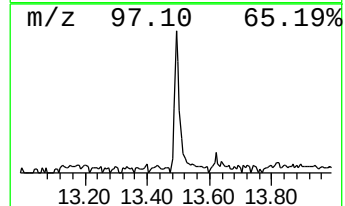
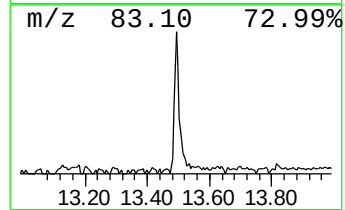
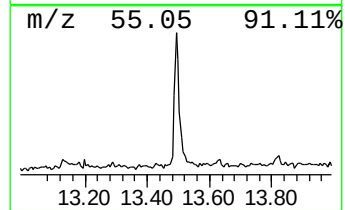
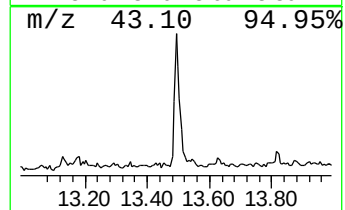
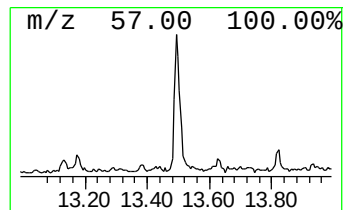
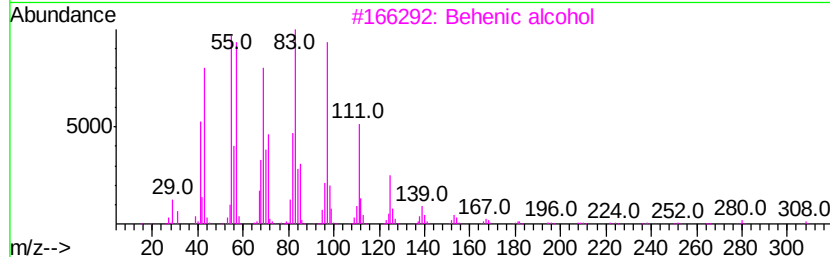
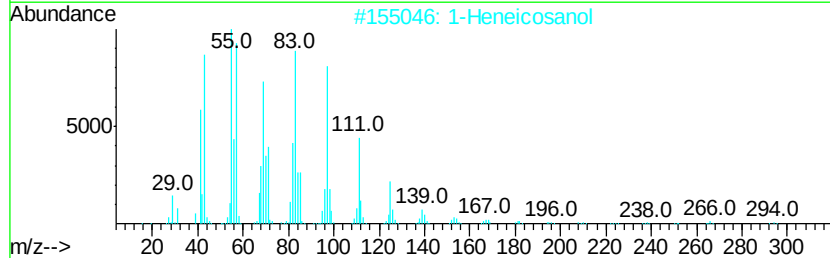
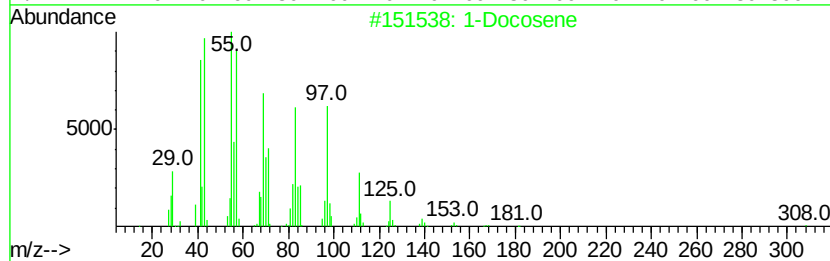
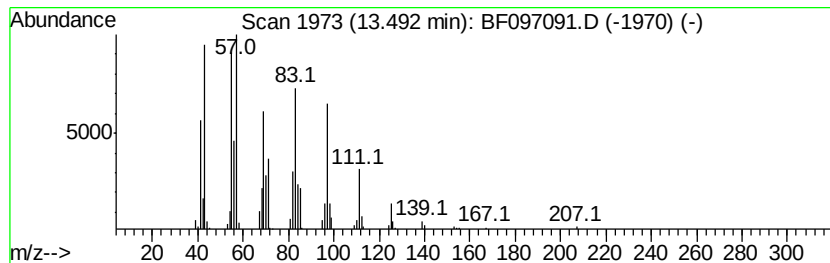
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	6.04 ng	189985	Chrysene-d12	13.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



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295-N-5-(0-2)

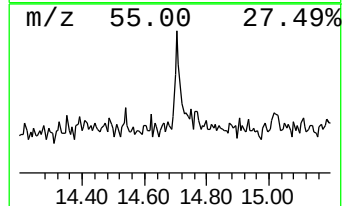
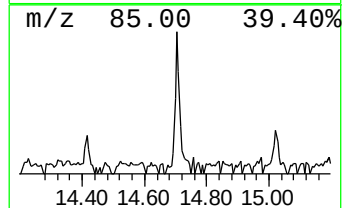
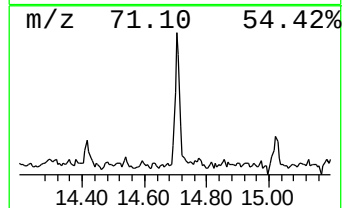
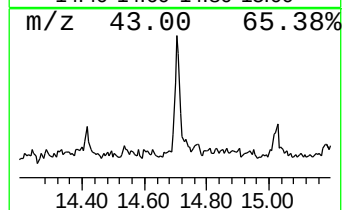
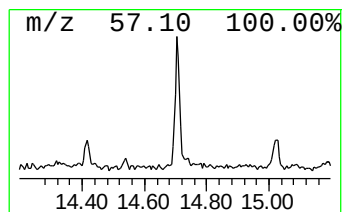
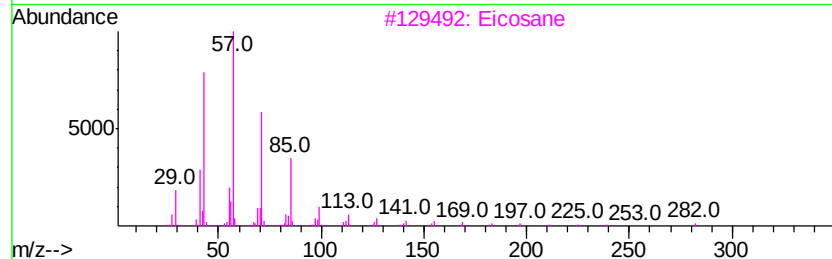
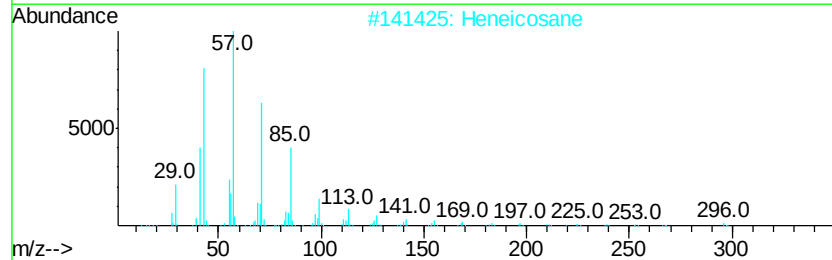
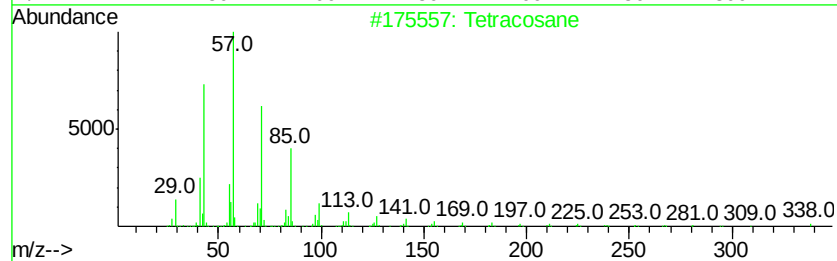
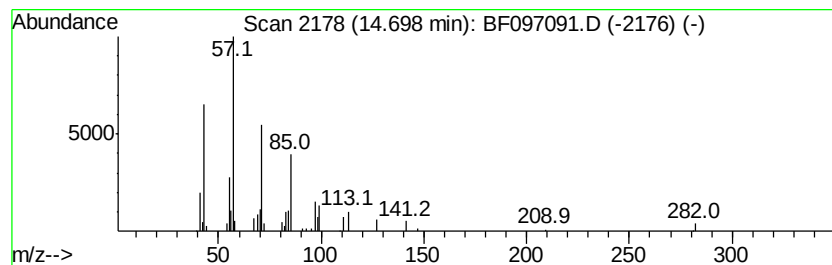
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	3.40 ng	87036	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane	282	C20H42	000112-95-8	90
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097091.D
Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
Sample : I4360-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
295-N-5-(0-2)

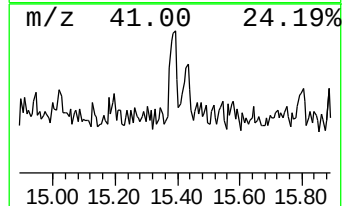
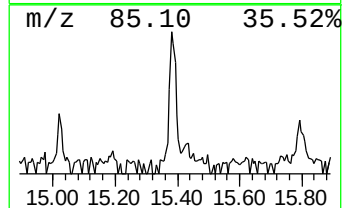
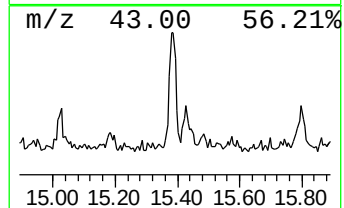
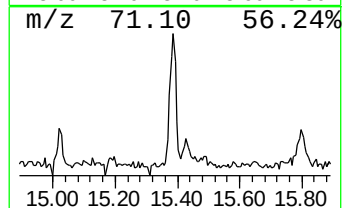
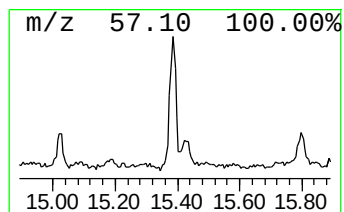
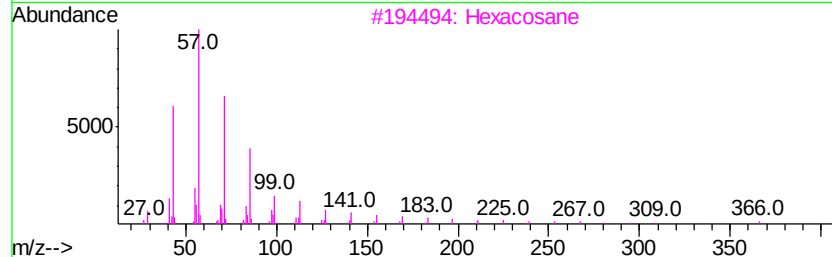
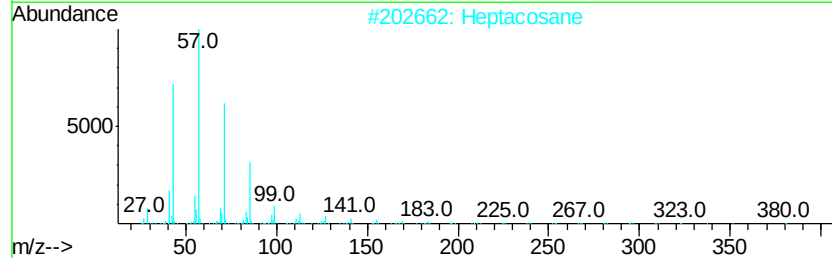
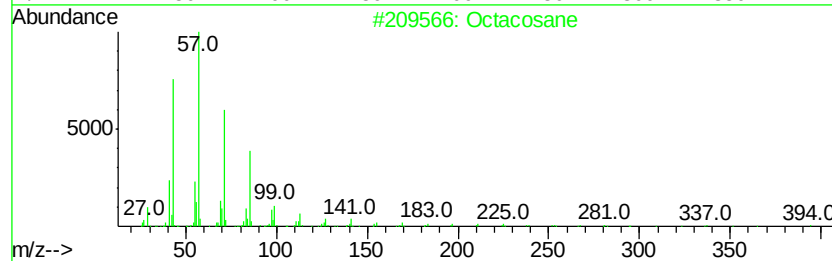
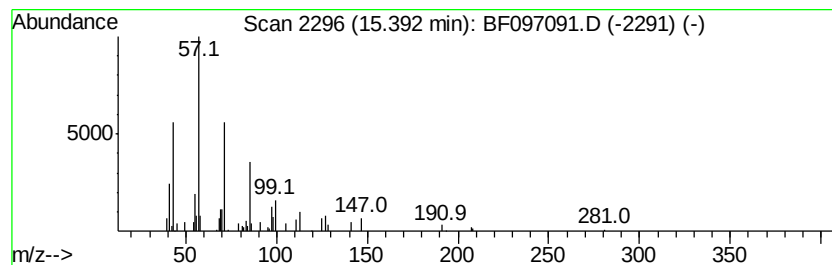
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	2.68 ng	68713	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Heptacosane	380	C27H56	000593-49-7	72
3		Hexacosane	366	C26H54	000630-01-3	68
4		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	64
5		triacontane	422	C30H62	000638-68-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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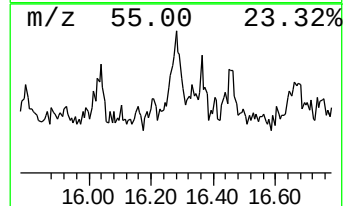
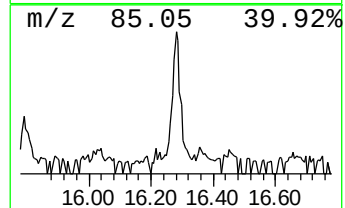
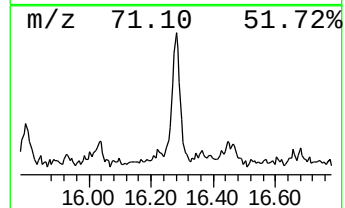
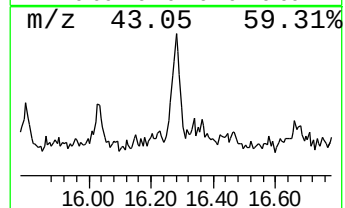
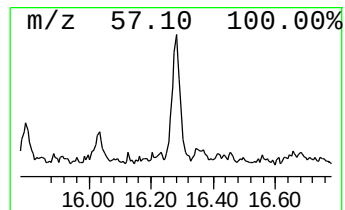
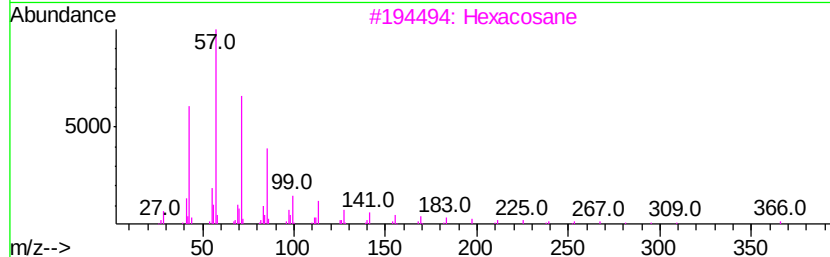
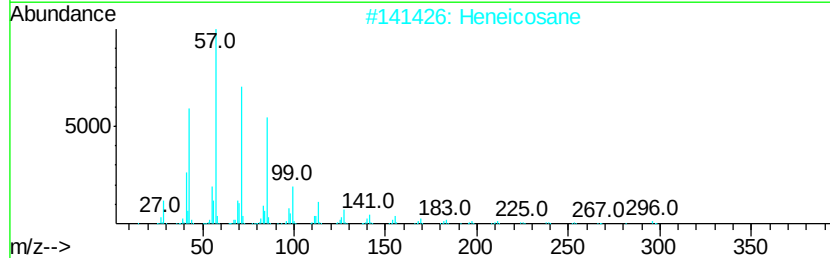
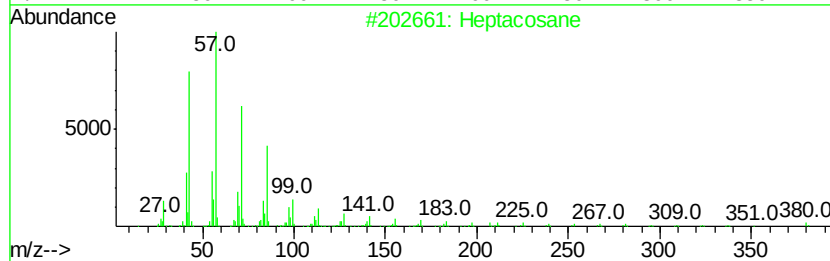
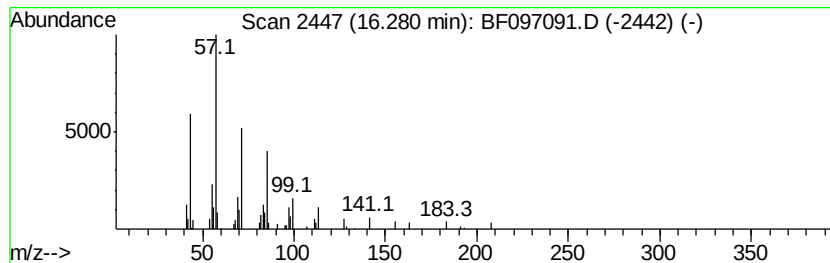
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	2.67 ng	68444	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097091.D
Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
Sample : I4360-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
295-N-5-(0-2)

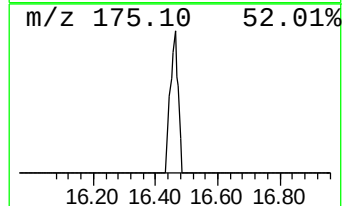
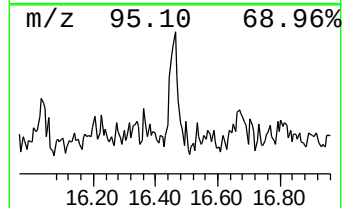
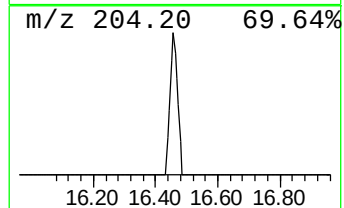
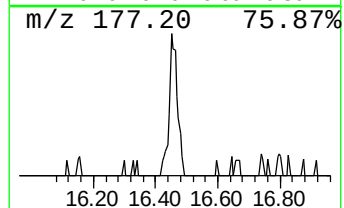
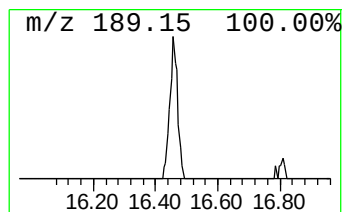
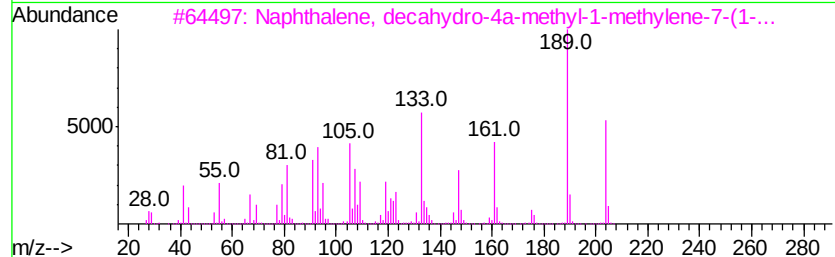
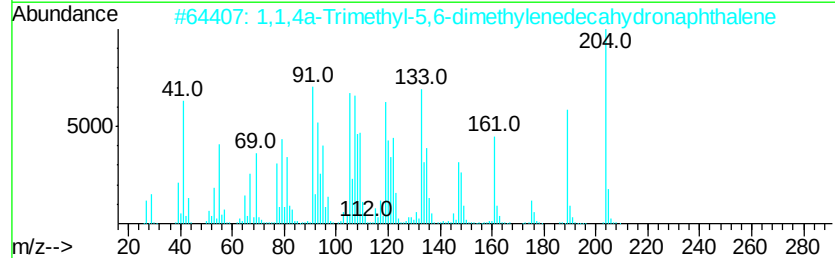
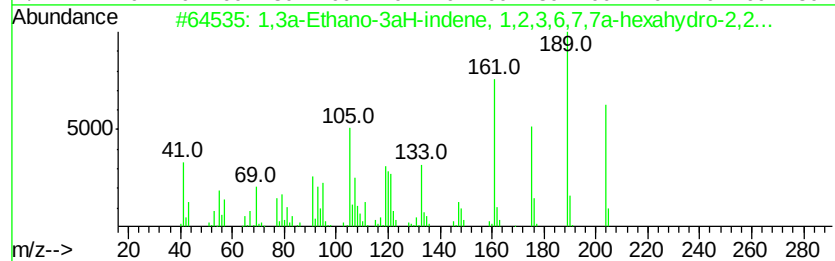
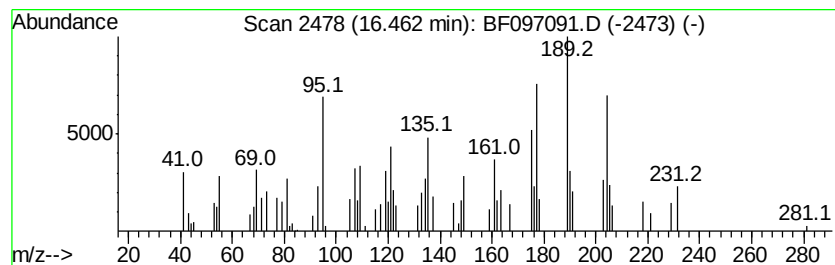
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.46 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.98 ng	76401	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	46
2		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	45
3		Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	41
4		.delta.-Selinene	204	C15H24	028624-23-9	38
5		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097091.D
Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
Sample : I4360-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

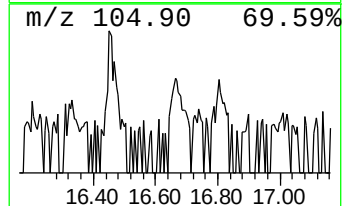
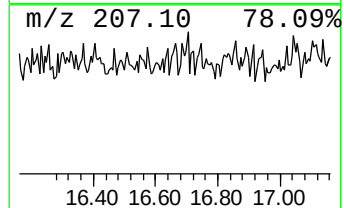
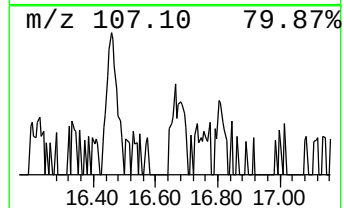
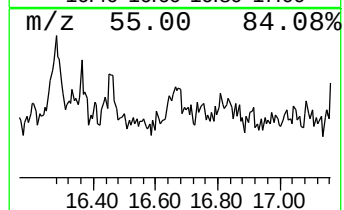
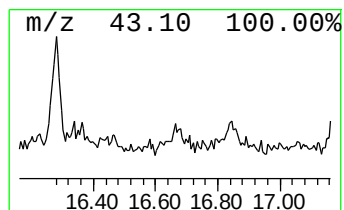
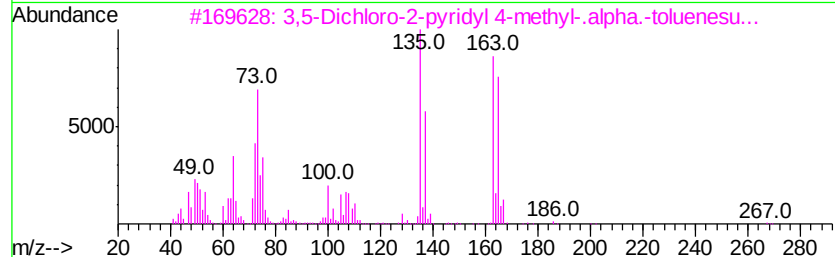
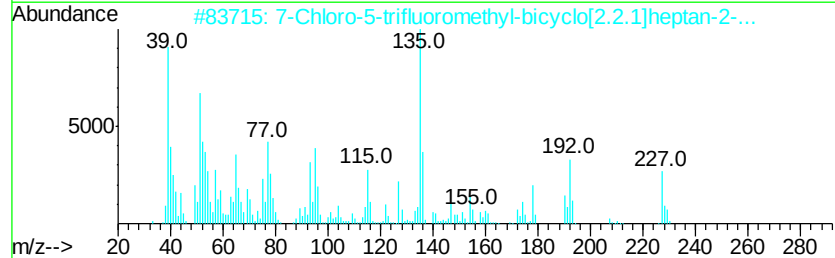
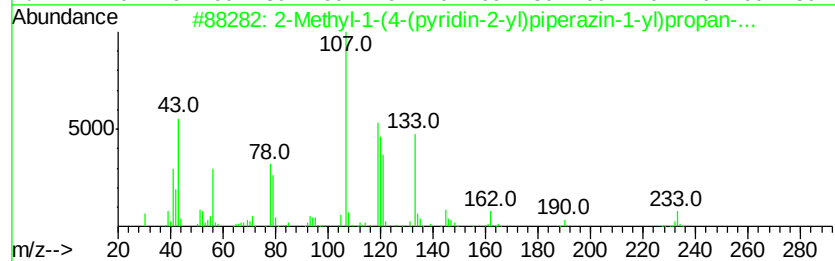
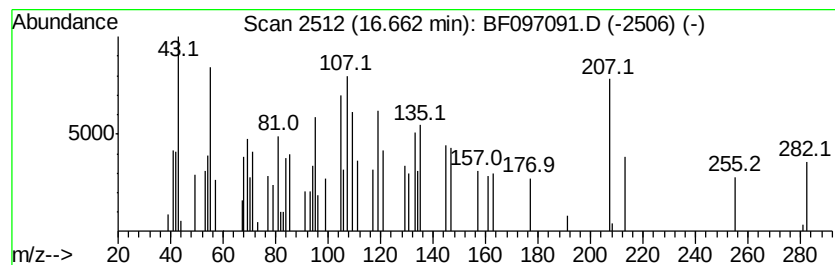
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.66 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.66	2.37 ng	60783	Perylene-d12	14.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-(4-(pyridin-2-yl)pipe...	233	C13H19N3O	1000368-48-5	14	
2	7-Chloro-5-trifluoromethyl-bicyc...	227	C8H9ClF3NO	1000278-15-7	11	
3	3,5-Dichloro-2-pyridyl 4-methyl-...	331	C13H11Cl2N03S	058236-59-2	10	
4	Propane, 1,1,1,3-tetrachloro-	180	C3H4Cl4	001070-78-6	10	
5	Anthranilic acid, N-methyl-, but...	207	C12H17N02	015236-34-7	10	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097091.D
Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
Sample : I4360-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
295-N-5-(0-2)

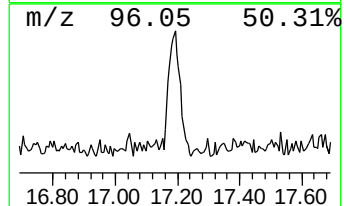
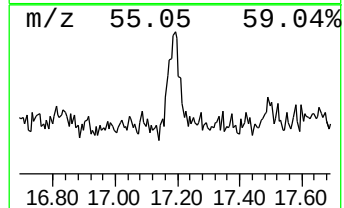
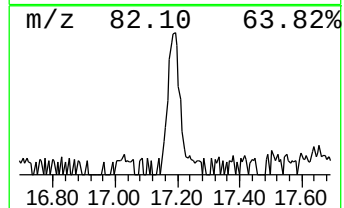
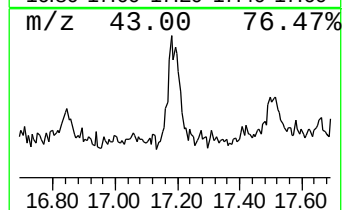
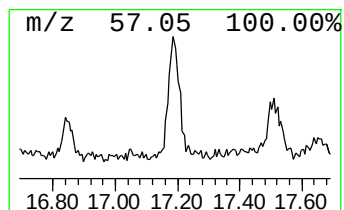
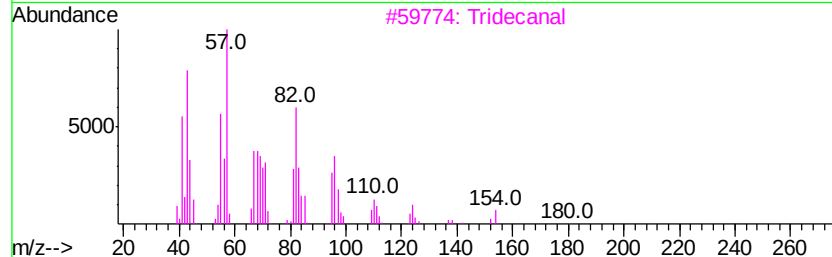
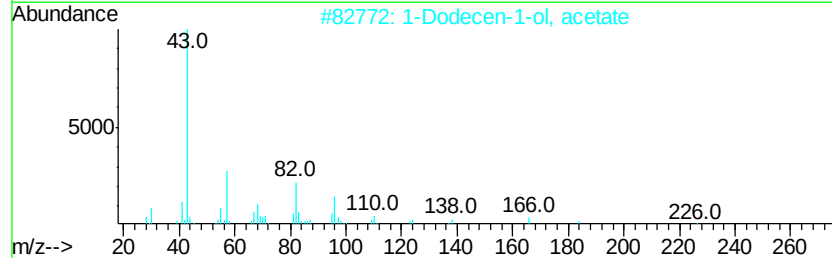
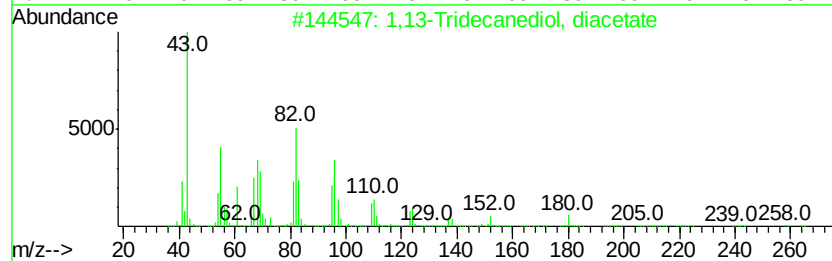
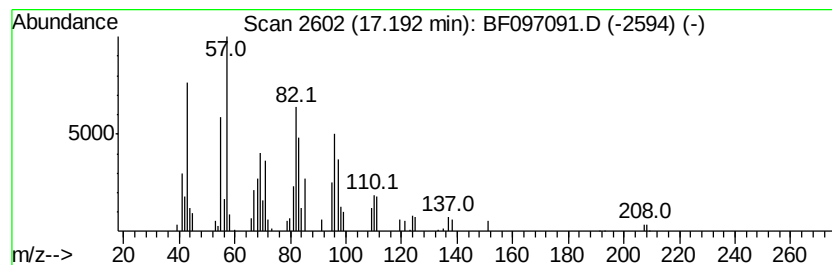
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,13-Tridecanediol, diacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	5.45 ng	139619	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	53
2			1-Dodecen-1-ol, acetate	226	C14H26O2	056438-08-5	50
3			Tridecanal	198	C13H26O	010486-19-8	50
4			Cyclododecanemethanol	198	C13H26O	001892-12-2	43
5			Cyclohexanol, 2,2-dimethyl-	128	C8H16O	001193-46-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097091.D
Acq On : 26 Jul 2017 22:38
Operator : SJ/JU
Sample : I4360-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
295-N-5-(0-2)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	4.65	11.1 ng		368811	1	6.49	666134	20.0
unknown6.27	6.27	79.3 ng		2641230	1	6.49	666134	20.0
Pentadecane	10.45	3.3 ng		131173	4	11.00	799161	20.0
1-Docosene	13.49	6.0 ng		189985	5	13.62	629168	20.0
Tetracosane	14.70	3.4 ng		87036	6	14.97	512660	20.0
Octacosane	15.39	2.7 ng		68713	6	14.97	512660	20.0
Heptacosane	16.28	2.7 ng		68444	6	14.97	512660	20.0
unknown16.46	16.46	3.0 ng		76401	6	14.97	512660	20.0
unknown16.66	16.66	2.4 ng		60783	6	14.97	512660	20.0
1,13-Tridecanedio...	17.19	5.5 ng		139619	6	14.97	512660	20.0