

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
 Data File : BF087266.D
 Acq On : 21 May 2016 12:02
 Operator : UM/SJ
 Sample : H3169-16
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-24-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-BF051716.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.701	8	10	46	rVB	2397311	4642924	99.90%	10.941%
2	4.684	269	271	286	rBV	281568	562747	12.11%	1.326%
3	5.141	309	311	329	rBV	3244940	3726619	80.19%	8.782%
4	6.227	403	406	408	rBV	3729088	3862461	83.11%	9.102%
5	6.330	413	415	417	rBV	3975638	4106566	88.36%	9.677%
6	6.559	433	435	441	rVB	692326	885688	19.06%	2.087%
7	6.707	446	448	451	rBV	3025253	2814119	60.55%	6.632%
8	7.130	483	485	488	rBV	2336663	2426732	52.22%	5.719%
9	7.290	497	499	502	rBV	29460	54351	1.17%	0.128%
10	7.839	545	547	550	rBV	1052367	1210438	26.04%	2.852%
11	8.925	639	642	644	rBV	4727123	4647490	100.00%	10.952%
12	9.325	675	677	681	rBV	744301	640840	13.79%	1.510%
13	9.530	693	695	698	rBV	109644	117843	2.54%	0.278%
14	9.588	698	700	703	rVV	1575897	1397672	30.07%	3.294%
15	10.033	737	739	741	rVB	206561	167178	3.60%	0.394%
16	10.250	755	758	761	rBV	66946	107809	2.32%	0.254%
17	10.376	767	769	772	rBV	2496288	2610593	56.17%	6.152%
18	10.502	778	780	787	rVB	238503	295436	6.36%	0.696%
19	10.696	795	797	799	rBV	31054	48479	1.04%	0.114%
20	10.948	817	819	820	rBV	150976	132988	2.86%	0.313%
21	10.971	820	821	825	rVV	42041	47477	1.02%	0.112%
22	11.062	827	829	832	rVV	1335792	1339337	28.82%	3.156%
23	11.131	832	835	839	rVB	23256	56419	1.21%	0.133%
24	11.371	854	856	858	rVB	73025	58281	1.25%	0.137%
25	11.611	875	877	885	rBV2	29151	62499	1.34%	0.147%
26	12.479	951	953	956	rBV	108123	94275	2.03%	0.222%
27	12.651	965	968	970	rBV	4117014	4130988	88.89%	9.735%
28	13.177	1012	1014	1016	rBV	42591	48769	1.05%	0.115%
29	13.577	1043	1049	1055	rBV2	43227	143015	3.08%	0.337%
30	13.691	1055	1059	1066	rVB	1040515	1179236	25.37%	2.779%
31	14.525	1129	1132	1134	rBV	93242	84663	1.82%	0.200%
32	15.040	1175	1177	1187	rBV	564567	730626	15.72%	1.722%

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SB-24-COMP

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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

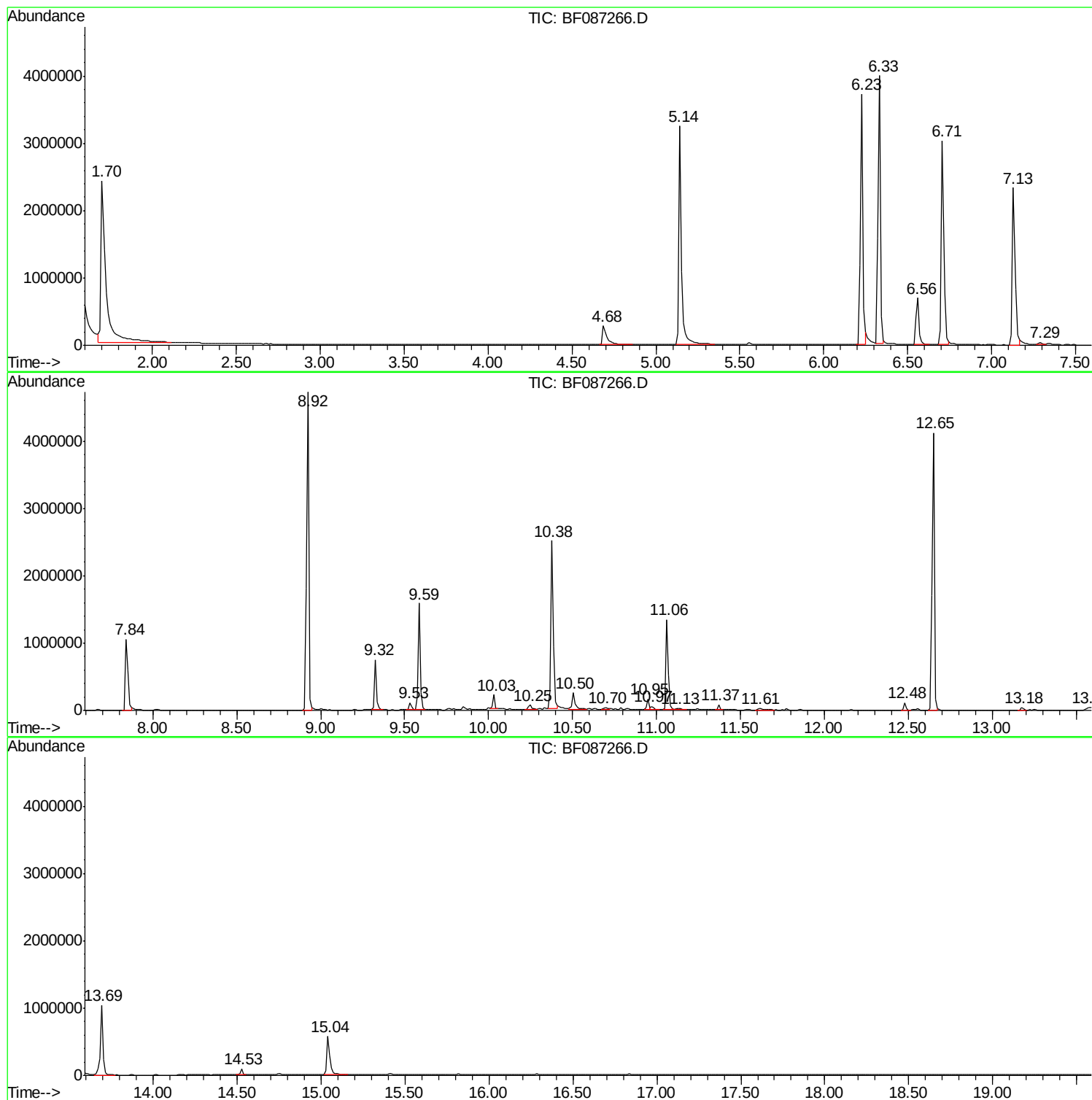
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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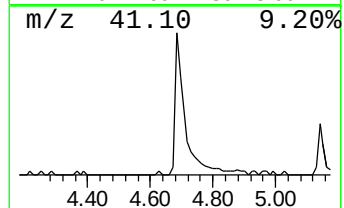
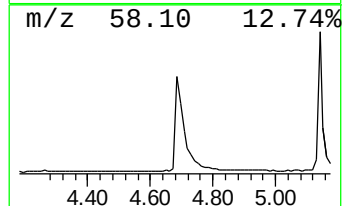
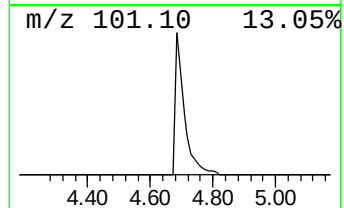
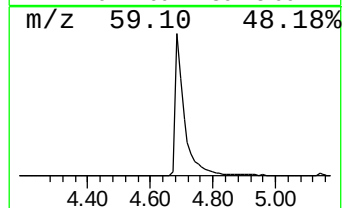
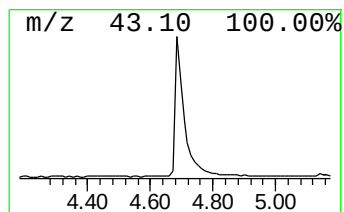
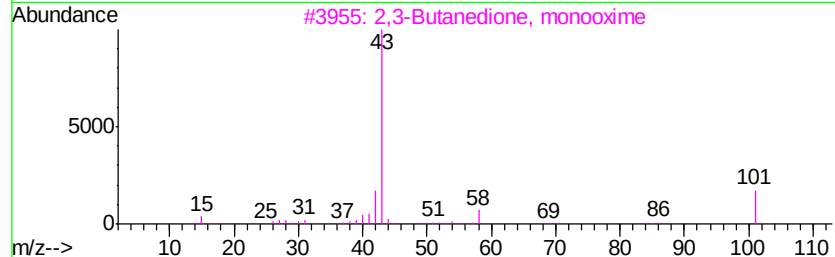
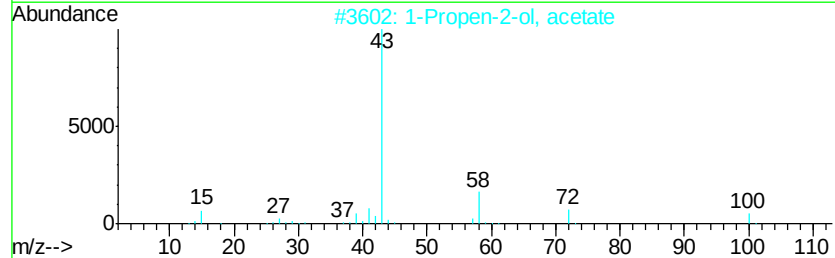
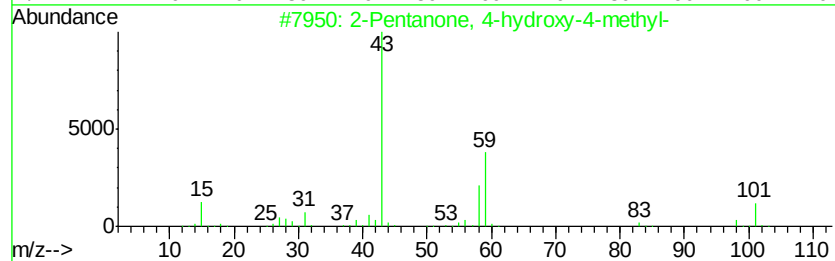
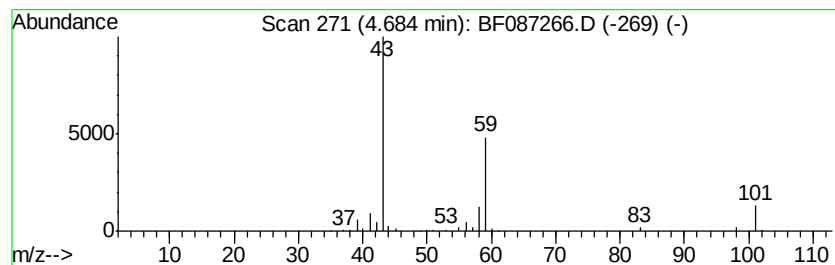
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.68	12.71 ng	562747	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane	58	C4H10	000106-97-8	9
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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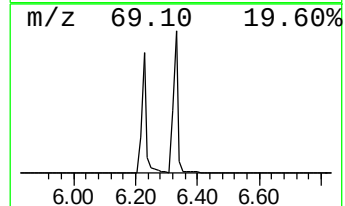
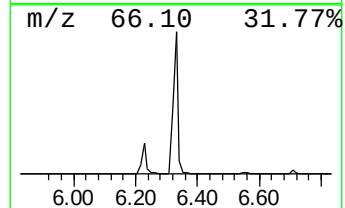
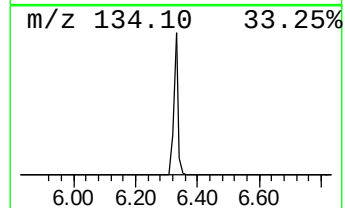
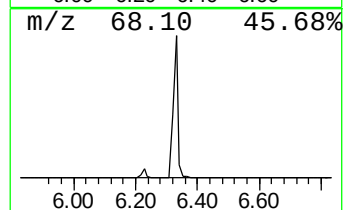
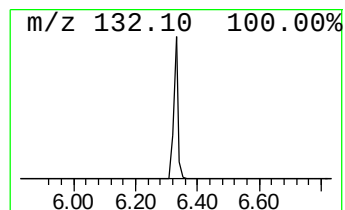
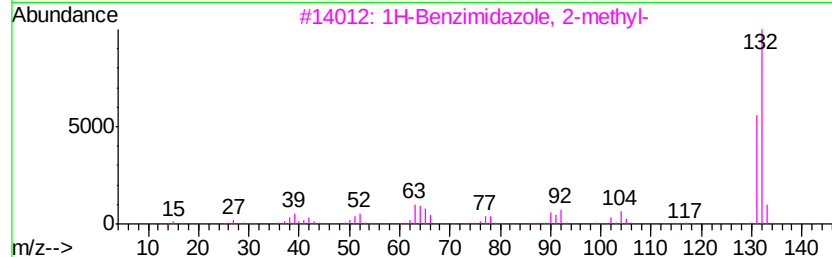
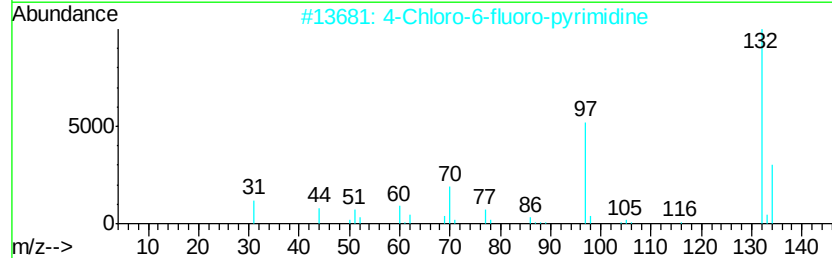
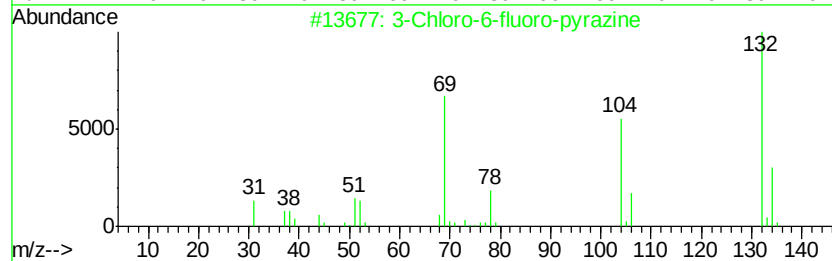
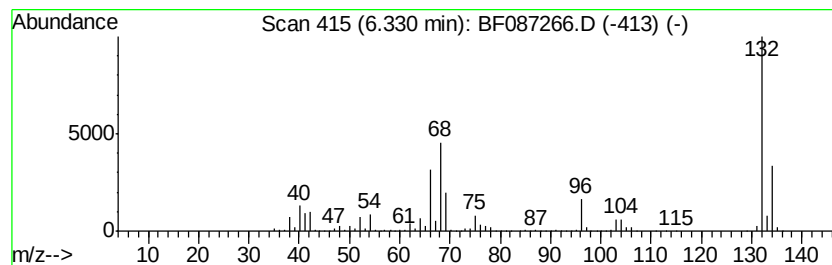
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	92.73 ng	4106570	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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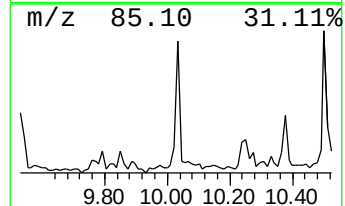
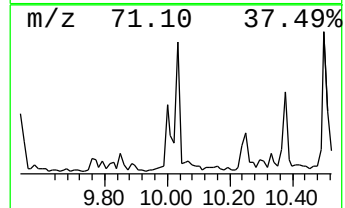
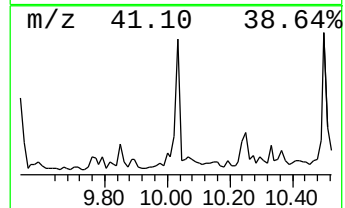
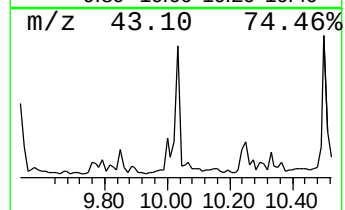
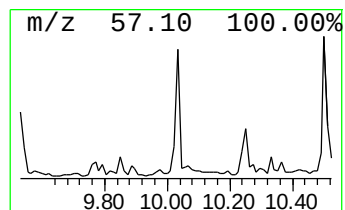
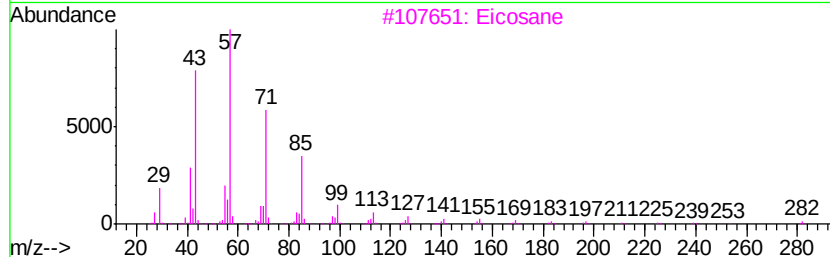
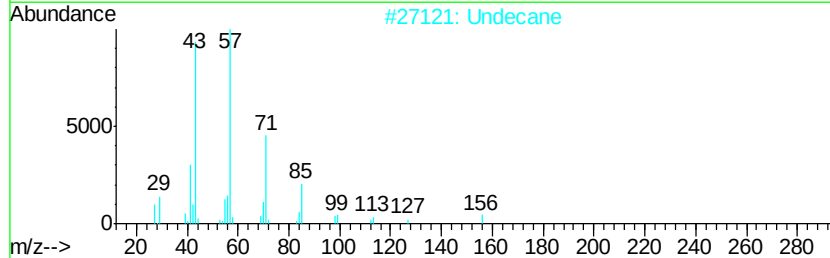
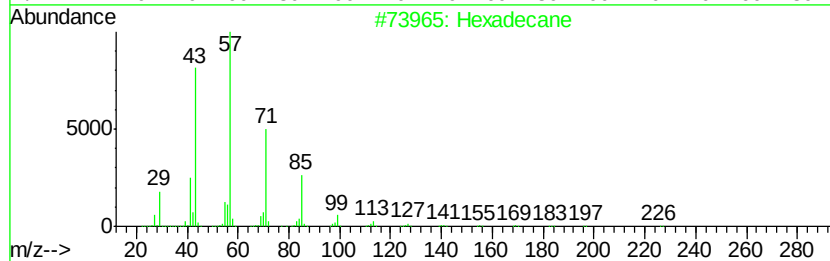
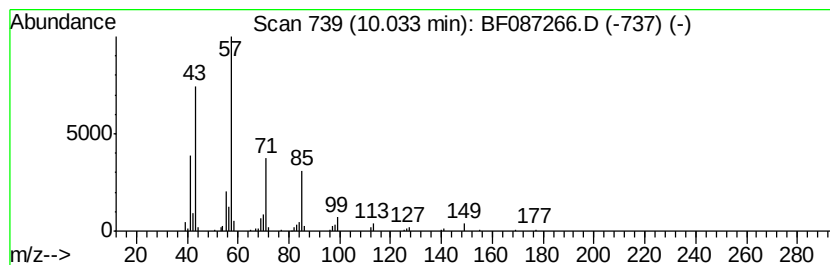
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.03	2.39 ng	167178	Acenaphthene-d10		9.59	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	90
2		Undecane	156	C11H24	001120-21-4	80
3		Eicosane	282	C20H42	000112-95-8	80
4		1-Iodoundecane	282	C11H23I	004282-44-4	72
5		Octadecane	254	C18H38	000593-45-3	72



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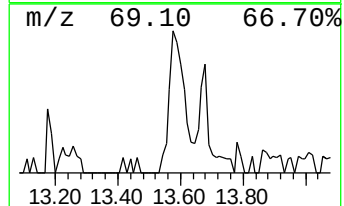
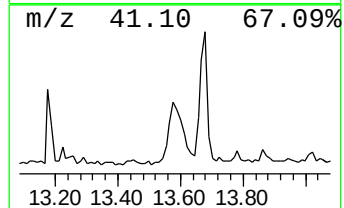
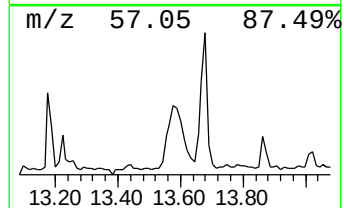
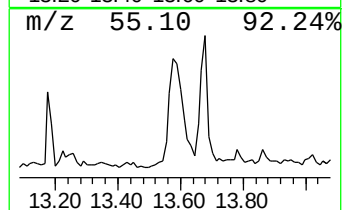
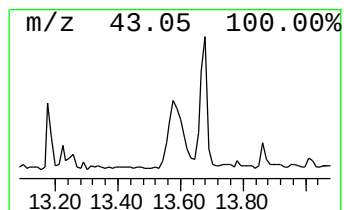
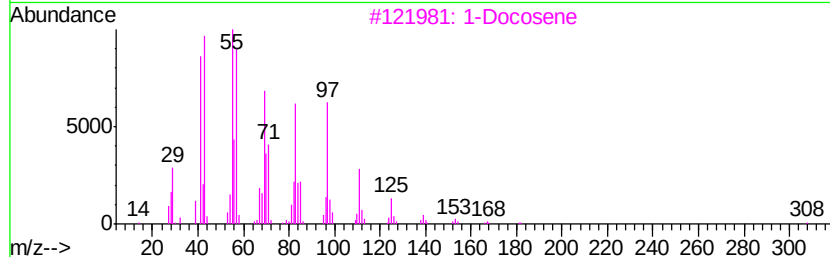
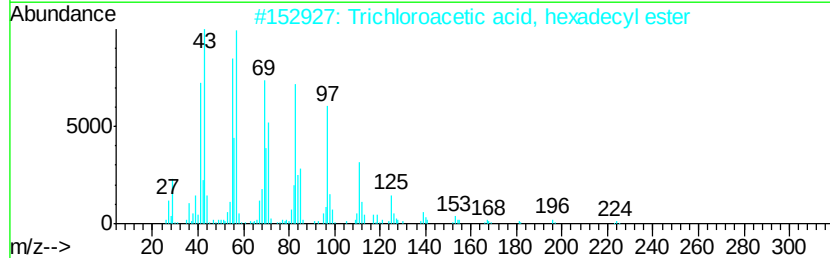
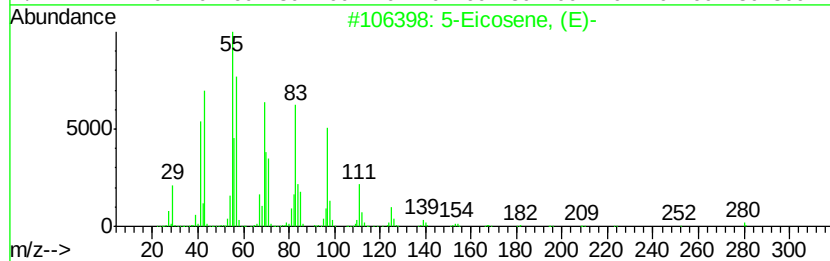
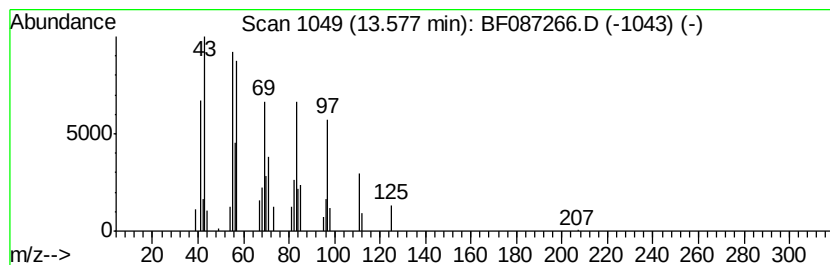
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.58	2.43 ng	143015	Chrysene-d12	13.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	11-Tricosene	322	C23H46	052078-56-5	91



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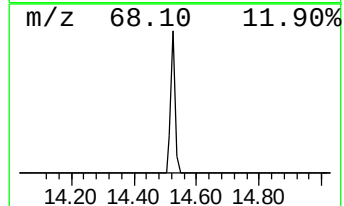
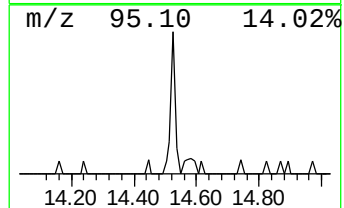
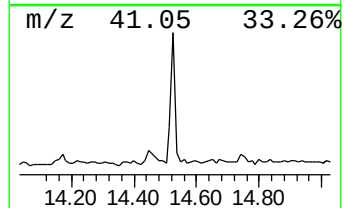
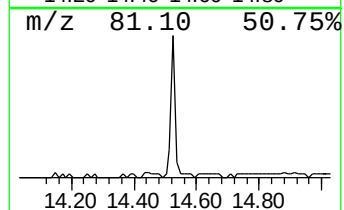
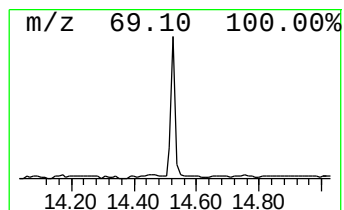
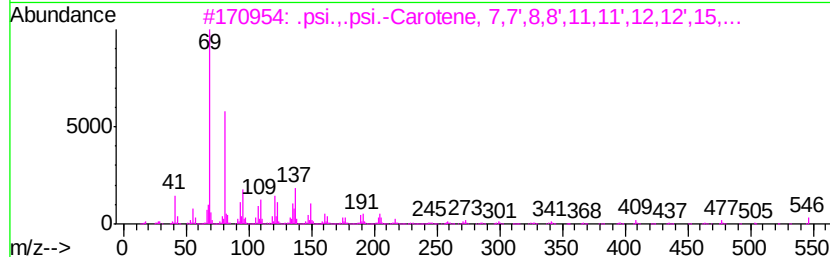
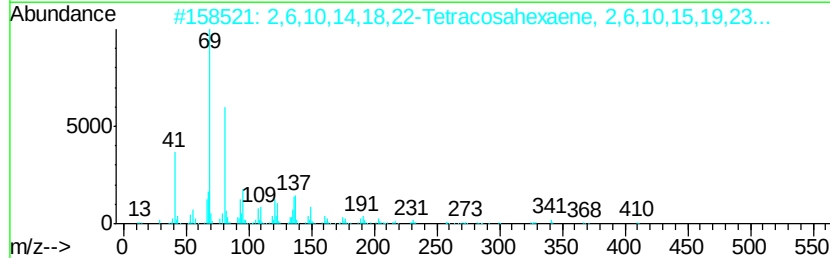
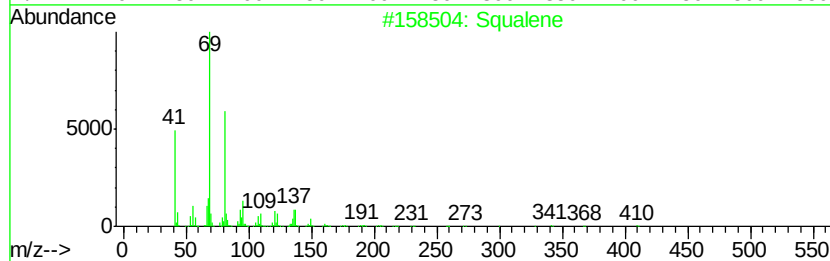
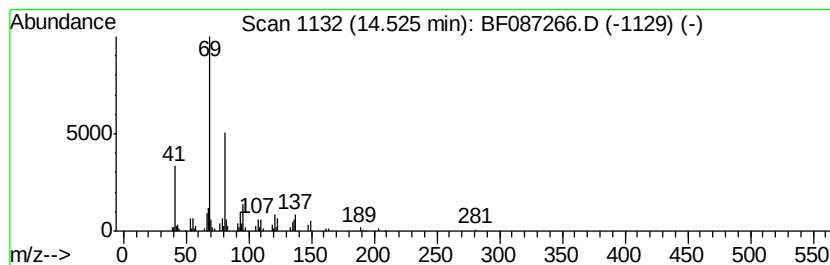
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.32 ng	84663	Perylene-d12	15.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
5		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	12.7	ng	562747	1	6.56	885688	20.0
unknown6.33	6.33	92.7	ng	4106570	1	6.56	885688	20.0
Hexadecane	10.03	2.4	ng	167178	3	9.59	1397670	20.0
5-Eicosene, (E)-	13.58	2.4	ng	143015	5	13.69	1179240	20.0
Squalene	14.53	2.3	ng	84663	6	15.04	730626	20.0