

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073016\
Data File : BF089445.D
Acq On : 30 Jul 2016 9:09
Operator : UM/SJ
Sample : H4215-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-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-BF072716.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	1.678	6	8	62	rVB	1038027	2508319	100.00%	18.162%
2	4.616	262	265	280	rBV	252068	430009	17.14%	3.114%
3	5.096	305	307	328	rBV	983010	1282581	51.13%	9.287%
4	6.181	399	402	409	rBV	1031732	1261097	50.28%	9.131%
5	6.284	409	411	423	rVB	1185395	1272954	50.75%	9.217%
6	6.513	429	431	438	rBV2	206297	240482	9.59%	1.741%
7	6.673	442	445	447	rBV	1122334	1045178	41.67%	7.568%
8	7.096	479	482	484	rBV	501783	717911	28.62%	5.198%
9	7.805	542	544	546	rBV	309944	294723	11.75%	2.134%
10	8.879	636	638	641	rBV	1241955	1321757	52.69%	9.570%
11	9.279	671	673	676	rBV	178155	154535	6.16%	1.119%
12	9.542	694	696	699	rBV	350035	316217	12.61%	2.290%
13	9.999	734	736	738	rBV	32872	25779	1.03%	0.187%
14	10.330	763	765	770	rBV	724472	696183	27.75%	5.041%
15	10.468	775	777	784	rVB	37009	45406	1.81%	0.329%
16	11.016	823	825	827	rBV	316174	275992	11.00%	1.998%
17	11.576	872	874	881	rBB	17662	25855	1.03%	0.187%
18	12.605	961	964	966	rBV	944986	1174048	46.81%	8.501%
19	13.508	1041	1043	1049	rVB	54076	82037	3.27%	0.594%
20	13.634	1051	1054	1060	rBV	273210	293715	11.71%	2.127%
21	14.548	1132	1134	1137	rVB	32511	33390	1.33%	0.242%
22	14.731	1146	1150	1157	rBV7	33343	104698	4.17%	0.758%
23	14.971	1169	1171	1174	rBV	168595	208162	8.30%	1.507%

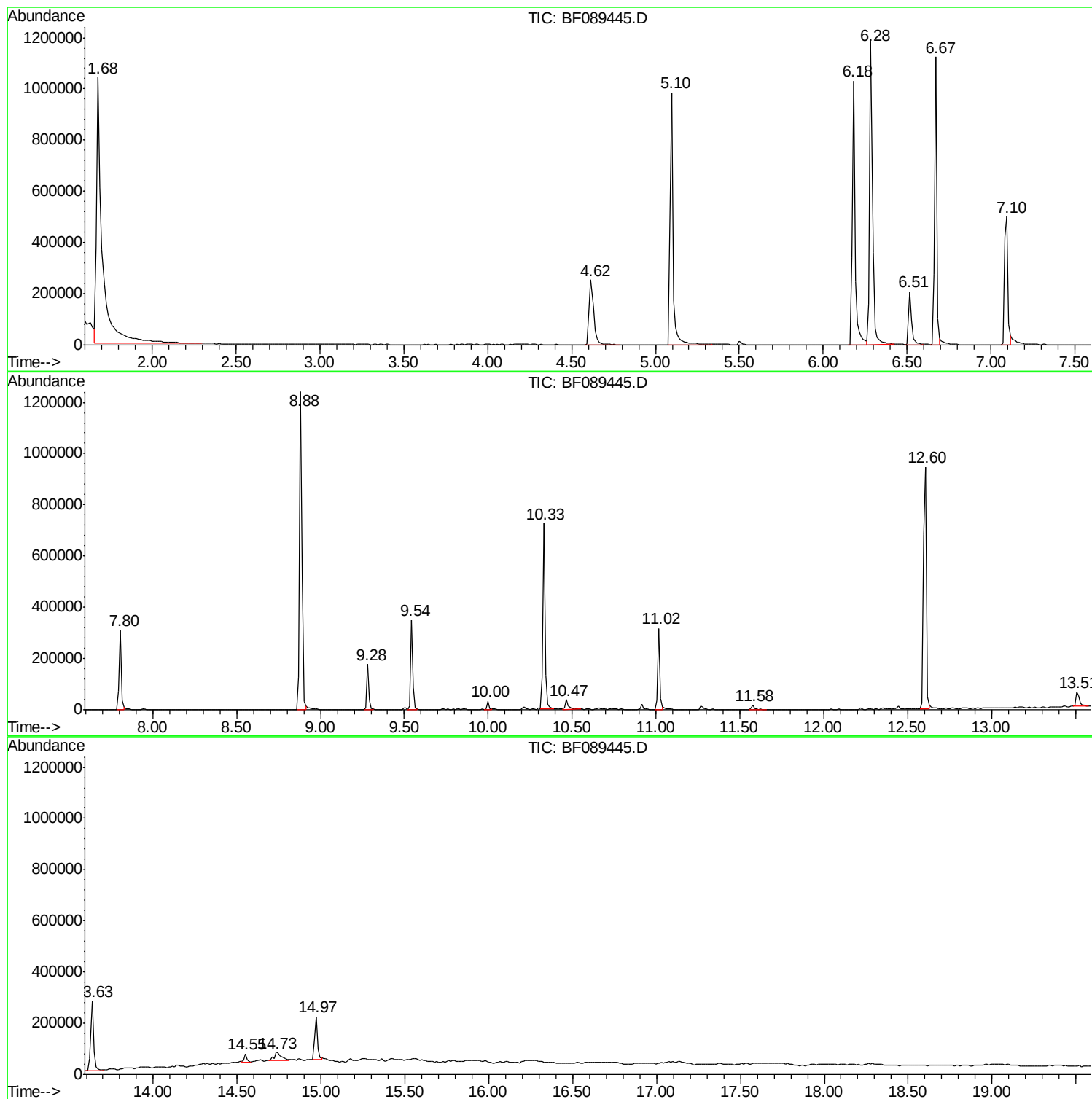
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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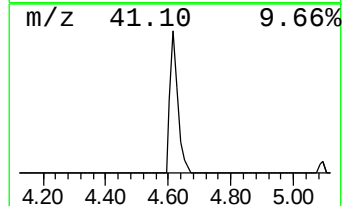
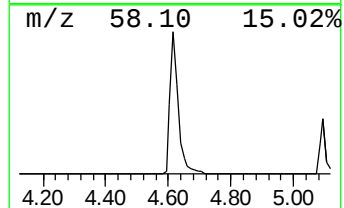
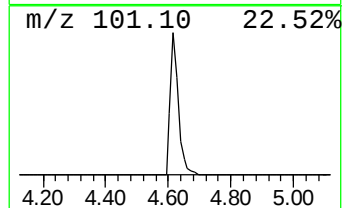
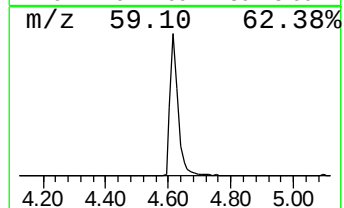
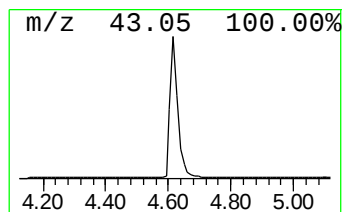
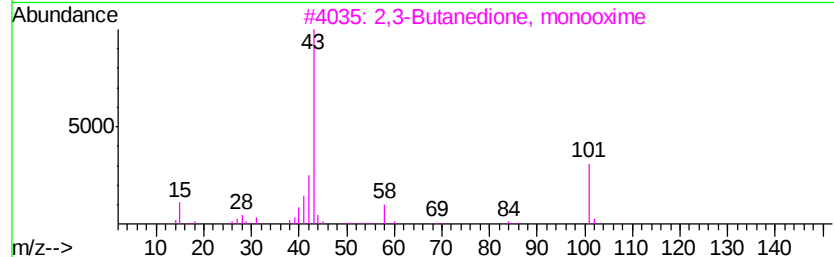
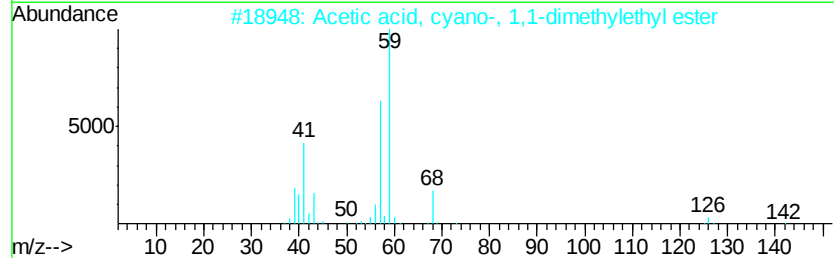
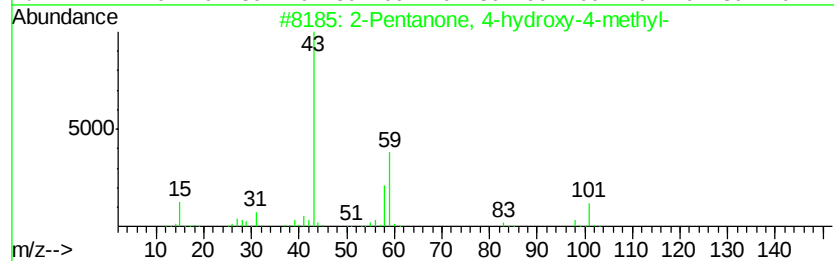
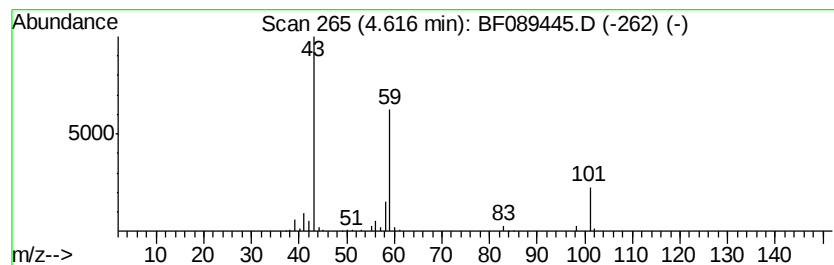
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	35.76 ng	430009	1,4-Dichlorobenzene-d4	6.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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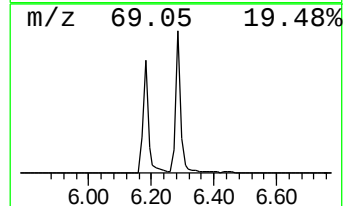
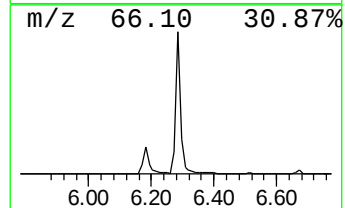
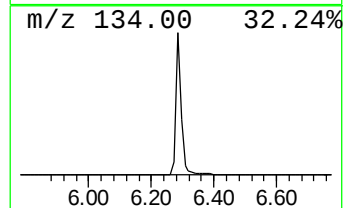
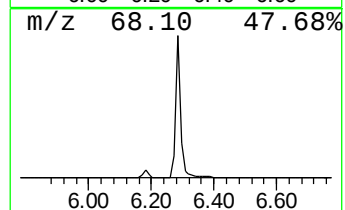
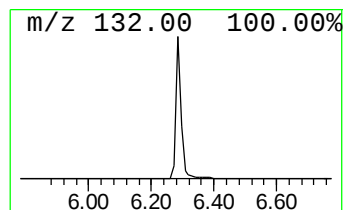
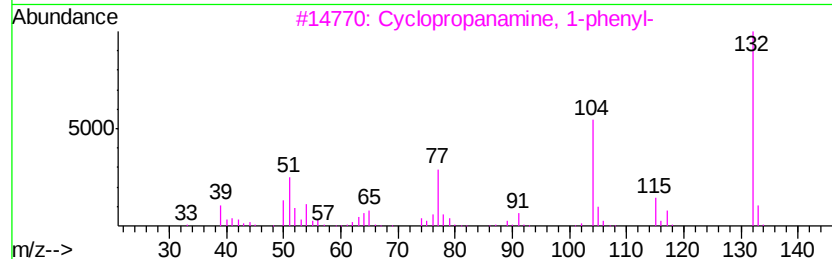
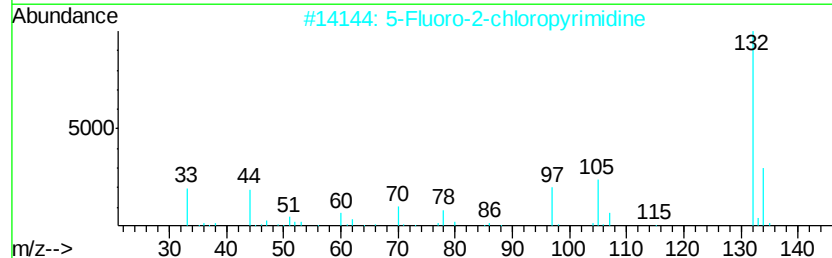
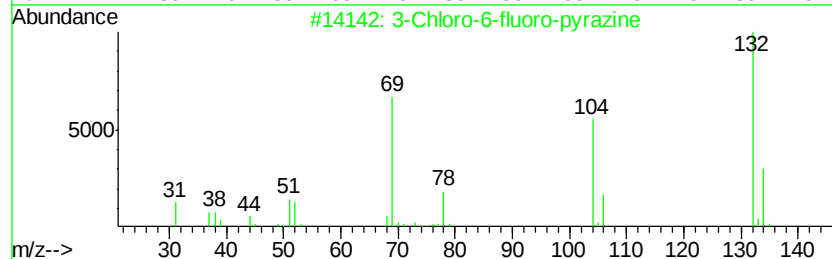
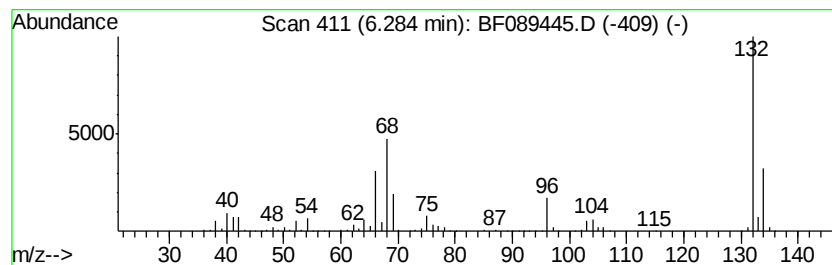
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Peak Number 3 unknown6.28 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.28	105.87 ng	1272950	1,4-Dichlorobenzene-d4	6.51

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	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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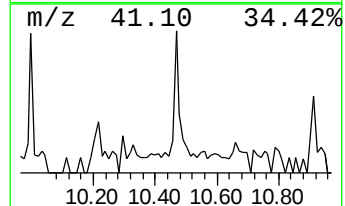
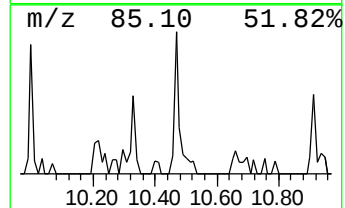
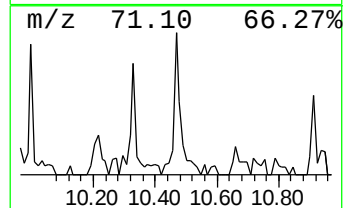
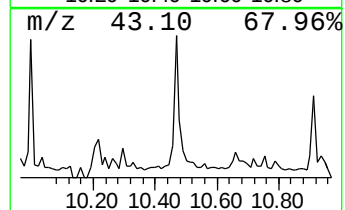
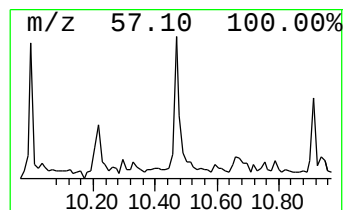
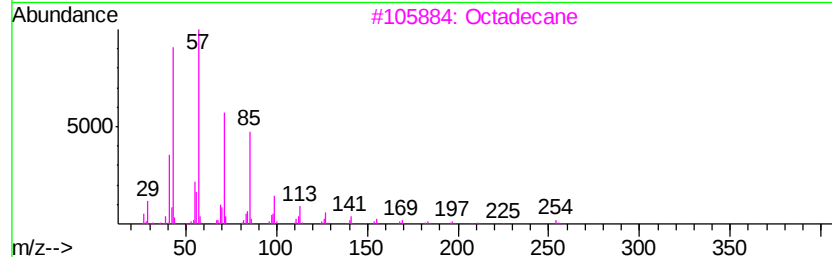
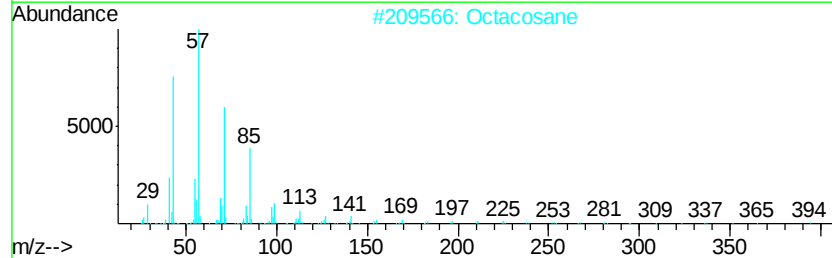
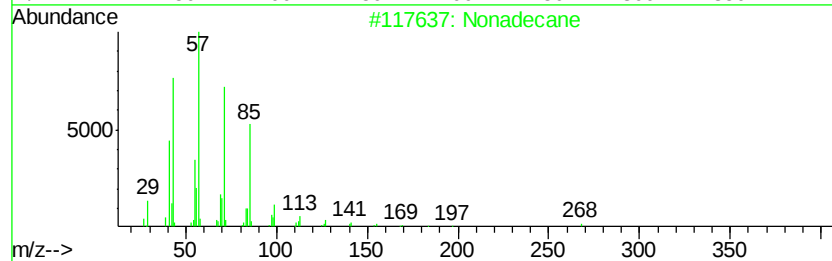
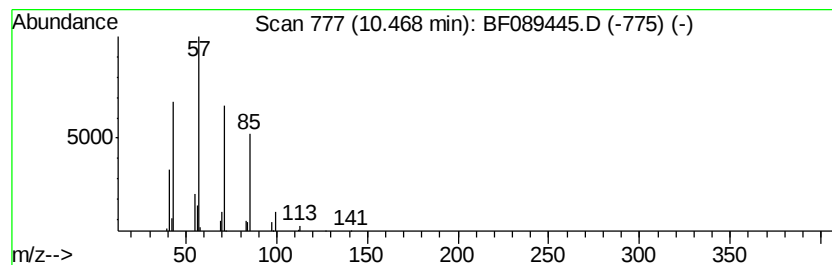
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Peak Number 5 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	3.29 ng	45406	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Octadecane		254	C18H38	000593-45-3	90
4	Tetradecane		198	C14H30	000629-59-4	90
5	Tritetracontane		605	C43H88	007098-21-7	90



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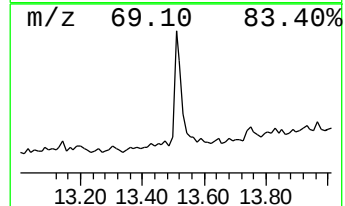
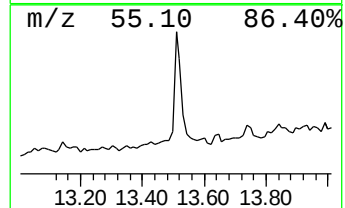
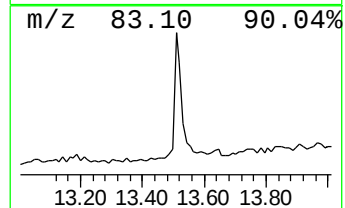
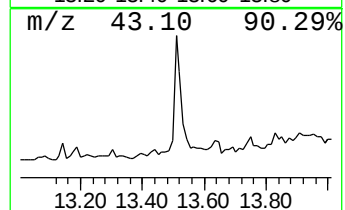
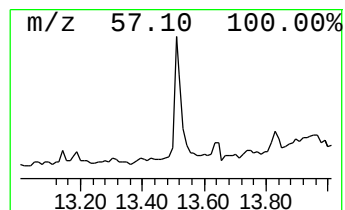
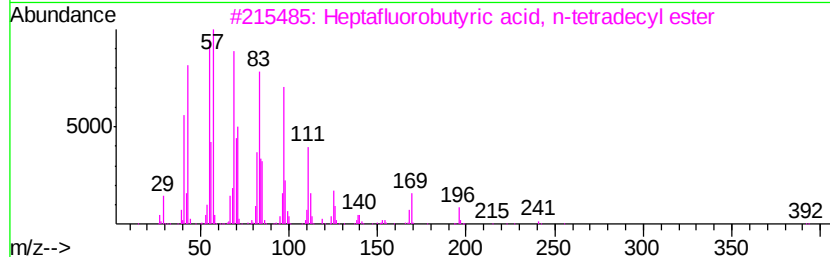
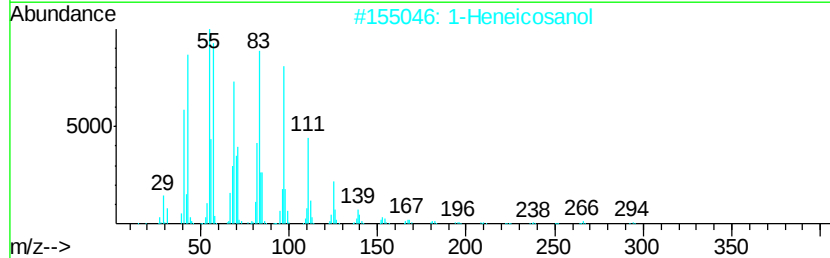
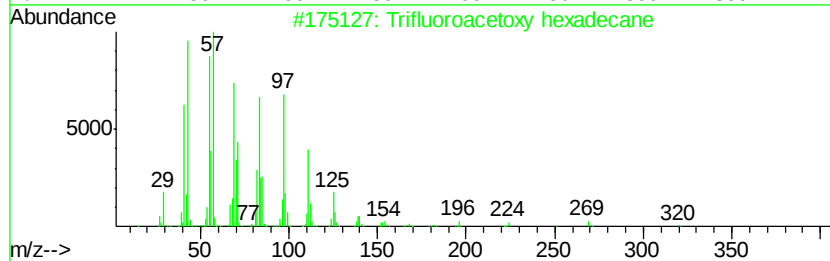
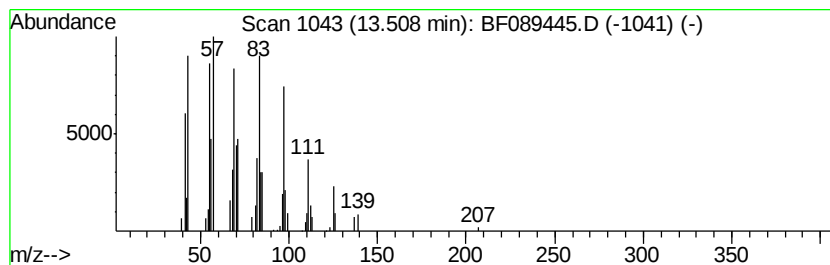
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	5.59 ng	82037	Chrysene-d12	13.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



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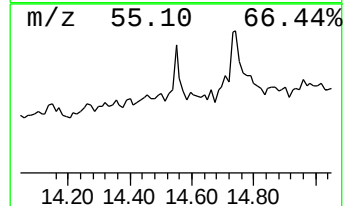
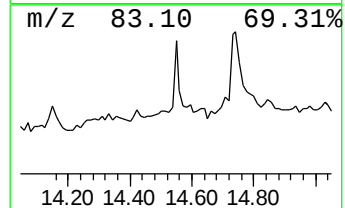
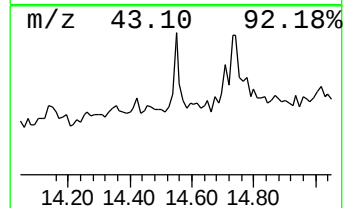
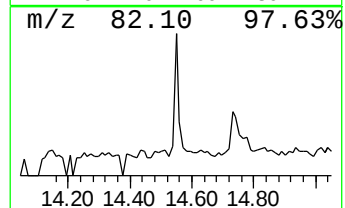
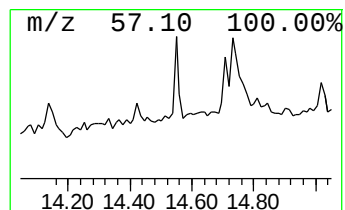
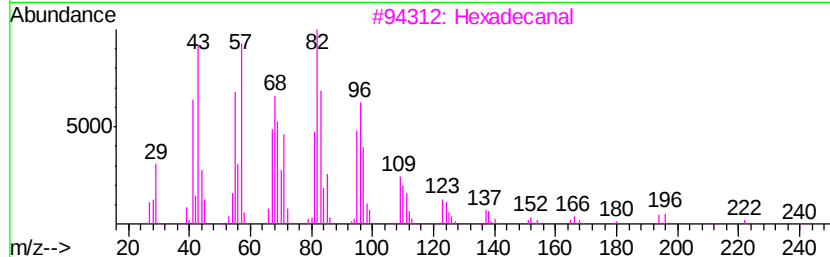
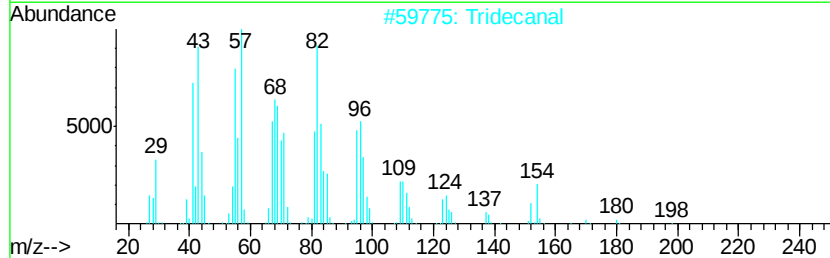
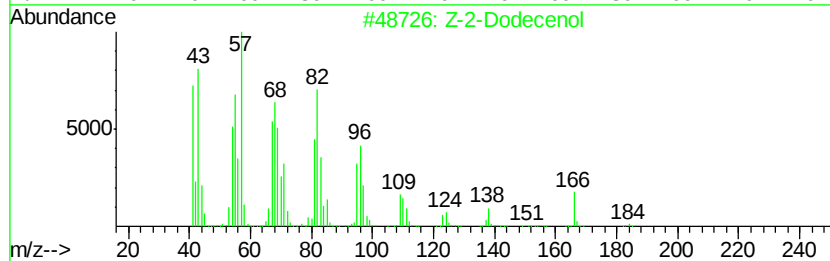
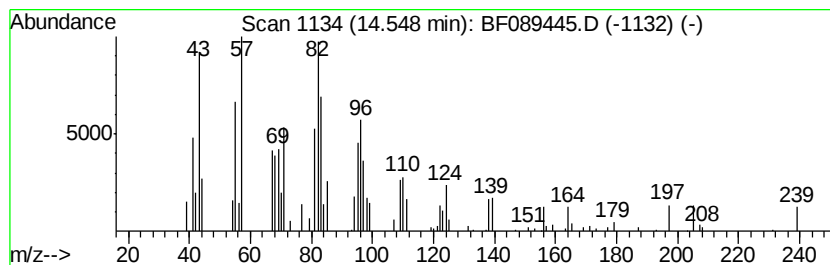
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Peak Number 7 Z-2-Dodecenol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.55	3.21 ng	33390	Perylene-d12		14.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-2-Dodecenol	184	C12H24O	069064-36-4	86
2	Tridecanal	198	C13H26O	010486-19-8	86
3	Hexadecanal	240	C16H32O	000629-80-1	80
4	17-Octadecenal	266	C18H34O	056554-86-0	80
5	Pentadecanal-	226	C15H30O	002765-11-9	72



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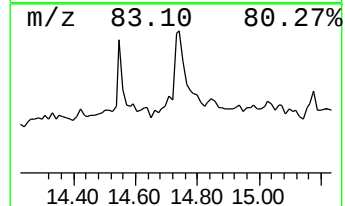
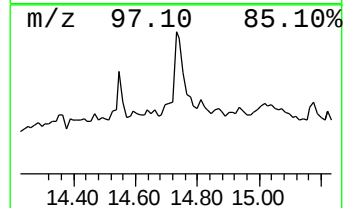
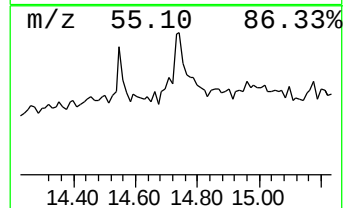
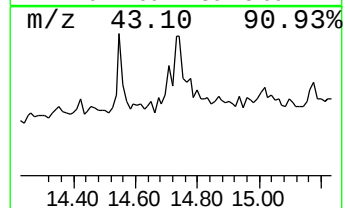
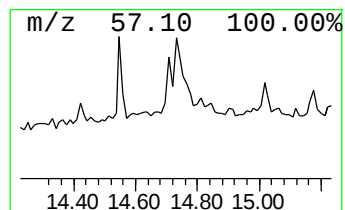
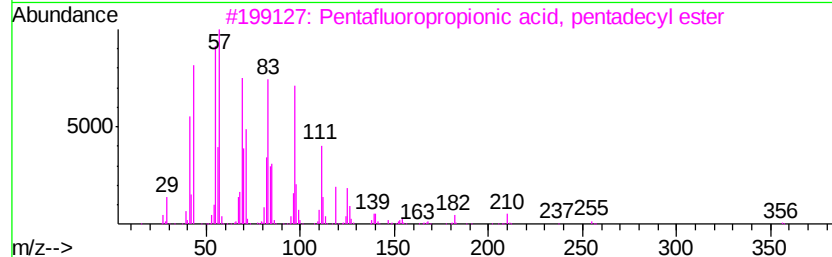
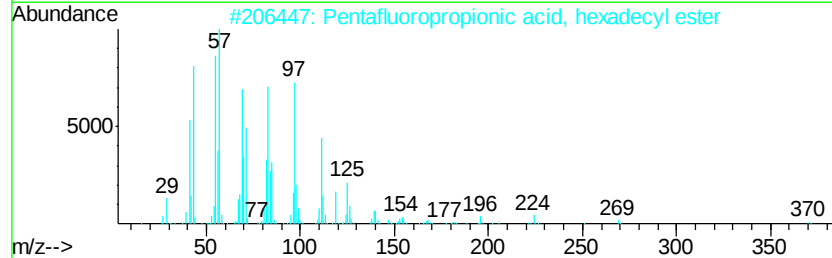
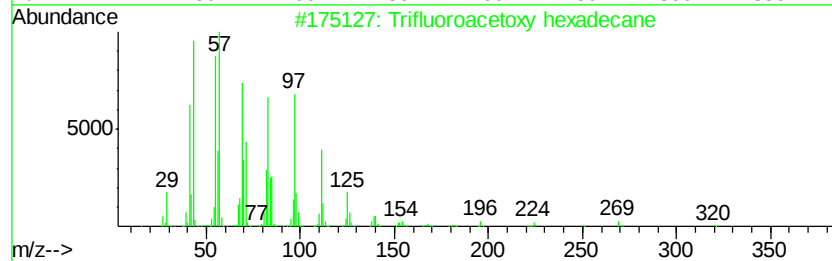
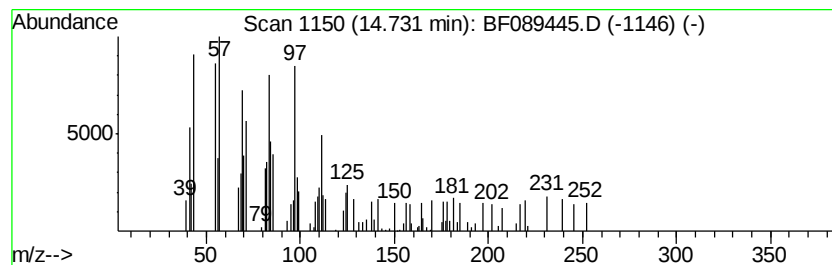
Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.73	10.06 ng	104698	Perylene-d12	14.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81
2		Pentafluoropropionic acid, hexadecanoic acid, 1,1,1,3,3,3-hexafluoro-	388	C19H33F5O2	006222-07-7	81
3		Pentafluoropropionic acid, pentadecanoic acid, 1,1,1,3,3,3-hexafluoro-	374	C18H31F5O2	959092-08-1	81
4		11-Tricosene	322	C23H46	052078-56-5	81
5		Heptafluorobutyric acid, pentadecanoic acid, 1,1,1,3,3,3,5,5,5-octafluoro-	424	C19H31F7O2	959261-23-5	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073016\
Data File : BF089445.D
Acq On : 30 Jul 2016 9:09
Operator : UM/SJ
Sample : H4215-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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
2-Pentanone, 4-hy...	4.62	35.8	ng	430009	1	6.51	240482	20.0
unknown6.28	6.28	105.9	ng	1272950	1	6.51	240482	20.0
Nonadecane	10.47	3.3	ng	45406	4	11.02	275992	20.0
Trifluoroacetoxy ...	13.51	5.6	ng	82037	5	13.63	293715	20.0
Z-2-Dodecenol	14.55	3.2	ng	33390	6	14.97	208162	20.0
Trifluoroacetoxy ...	14.73	10.1	ng	104698	6	14.97	208162	20.0