

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
 Data File : BF088766.D
 Acq On : 7 Jul 2016 6:44
 Operator : UM/SJ
 Sample : H3870-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-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-BF063016.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	9	10	17	rVB	47409	69387	1.47%	0.282%
2	1.827	19	21	32	rVB	486939	715184	15.10%	2.904%
3	4.913	288	291	296	rVB	97788	141168	2.98%	0.573%
4	5.336	326	328	331	rVB	1351691	1668806	35.24%	6.776%
5	6.387	417	420	422	rBV	1748684	1861754	39.31%	7.559%
6	6.513	428	431	434	rBV	1803694	1728249	36.49%	7.017%
7	6.742	449	451	453	rBV	396555	540417	11.41%	2.194%
8	6.902	463	465	467	rBB	1427400	1298383	27.41%	5.272%
9	7.313	498	501	503	rBV	1263425	1211763	25.59%	4.920%
10	8.033	561	564	566	rBV	928041	791883	16.72%	3.215%
11	9.108	656	658	661	rVB	1650460	1983590	41.88%	8.054%
12	9.508	691	693	695	rBV	281737	253865	5.36%	1.031%
13	9.782	715	717	719	rVV	926320	790950	16.70%	3.211%
14	10.571	783	786	788	rVV	925586	1051428	22.20%	4.269%
15	10.696	796	797	801	rBV	67339	82437	1.74%	0.335%
16	11.142	834	836	838	rBV	63294	57087	1.21%	0.232%
17	11.256	844	846	850	rVB	826204	744537	15.72%	3.023%
18	11.588	872	875	877	rVV2	46350	68707	1.45%	0.279%
19	11.668	880	882	885	rVB	1074986	898929	18.98%	3.650%
20	12.377	939	944	947	rBV2	2814116	4736140	100.00%	19.230%
21	12.457	949	951	954	rVB	502082	513592	10.84%	2.085%
22	12.685	968	971	974	rBV2	97182	118968	2.51%	0.483%
23	12.845	983	985	987	rVB	1794532	1636339	34.55%	6.644%
24	13.097	1004	1007	1013	rVB3	38786	91560	1.93%	0.372%
25	13.748	1063	1064	1071	rVB2	79157	102598	2.17%	0.417%
26	13.885	1073	1076	1077	rVV	500692	643211	13.58%	2.612%
27	14.377	1115	1119	1124	rBV2	23880	74822	1.58%	0.304%
28	14.674	1142	1145	1149	rVV3	39123	64786	1.37%	0.263%
29	14.880	1160	1163	1168	rVB	53804	120924	2.55%	0.491%
30	15.200	1189	1191	1194	rBV	35180	59599	1.26%	0.242%
31	15.268	1194	1197	1200	rBV	416511	507690	10.72%	2.061%

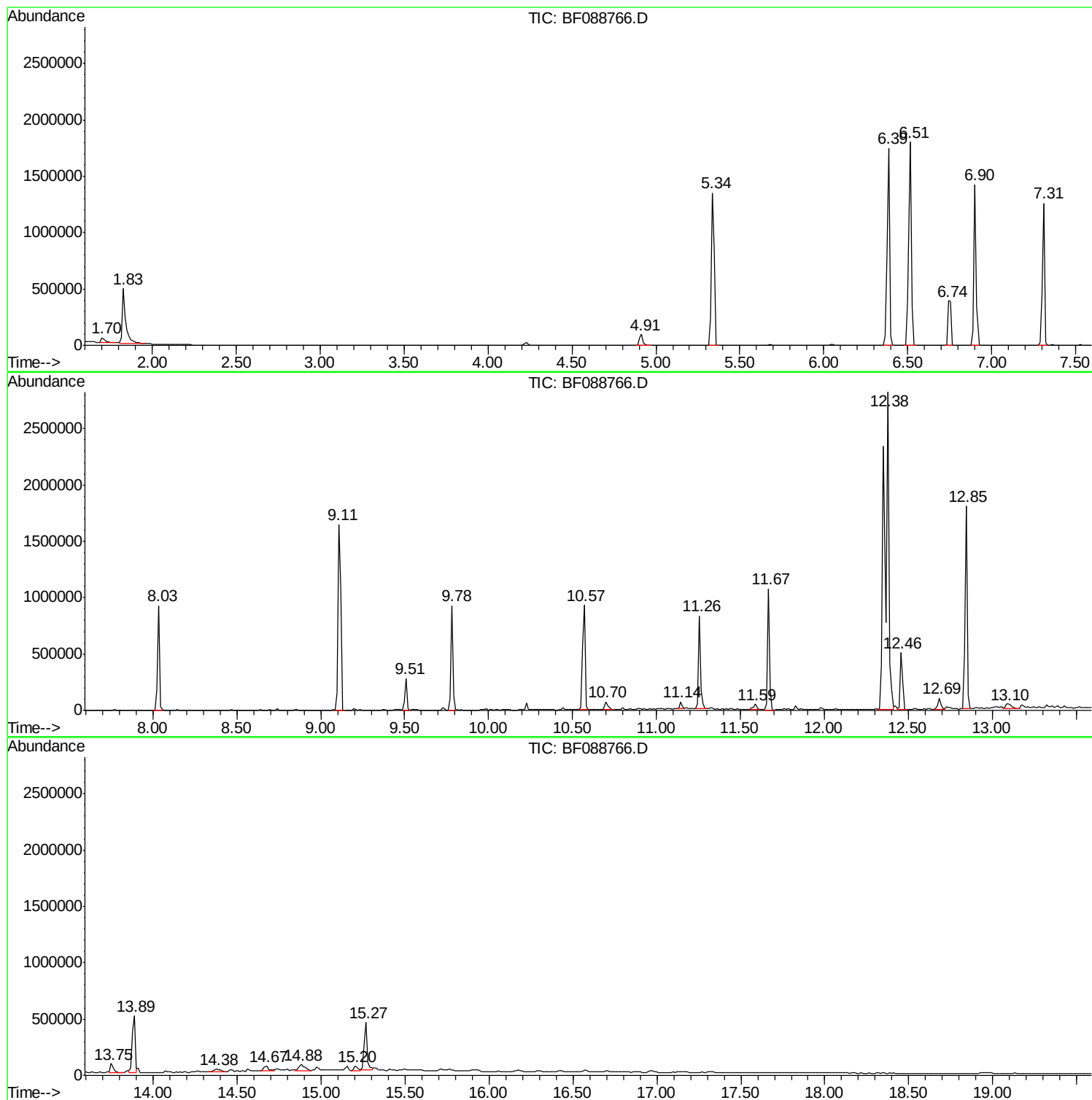
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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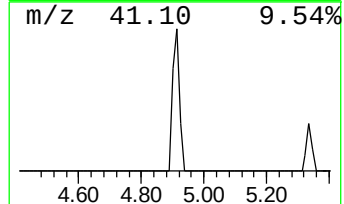
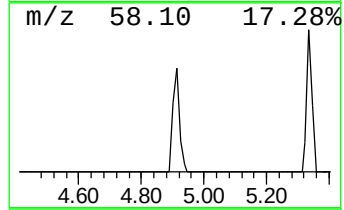
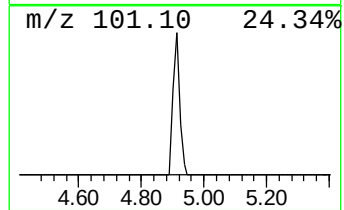
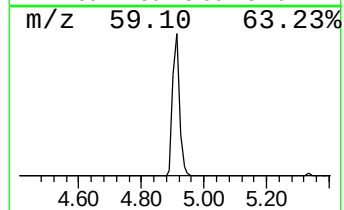
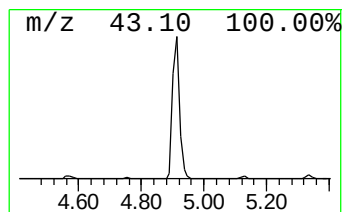
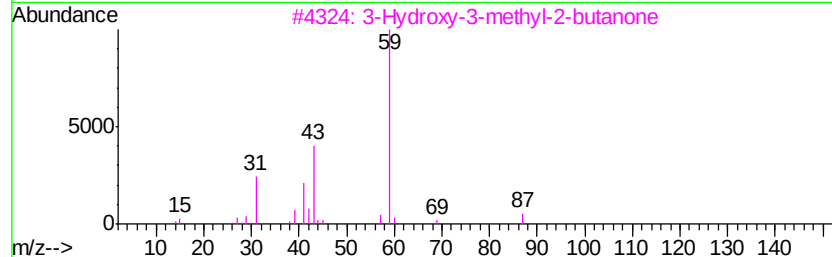
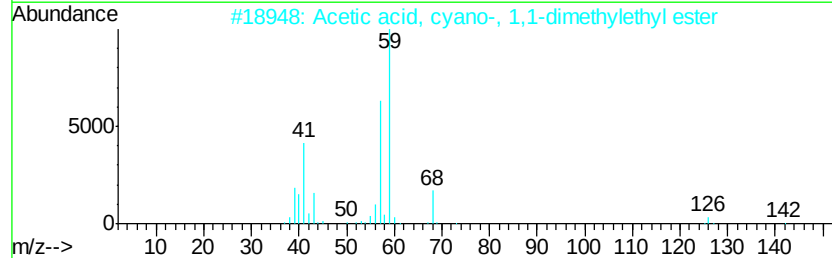
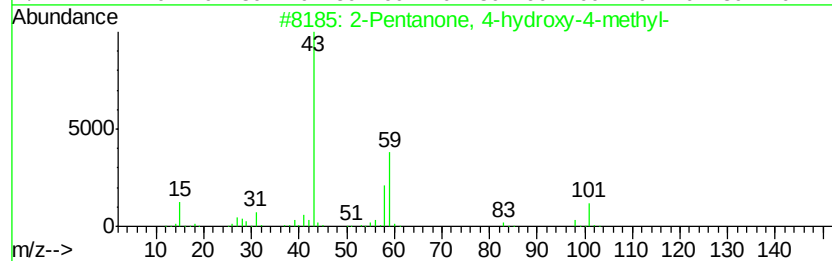
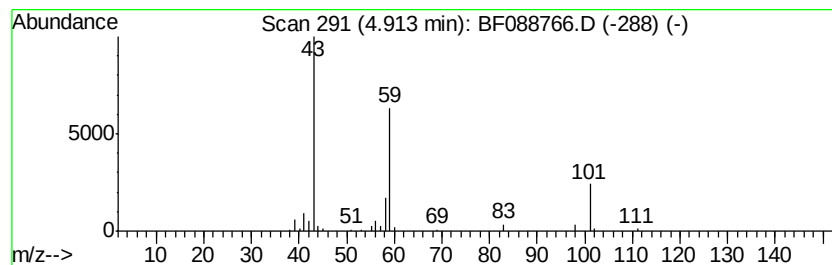
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	5.22 ng	141168	1,4-Dichlorobenzene-d4	6.75

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-dimethyl...	141	C7H11NO2	001116-98-9	17
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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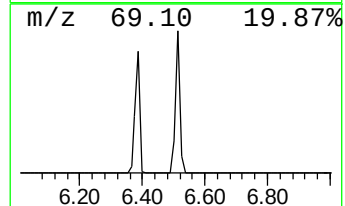
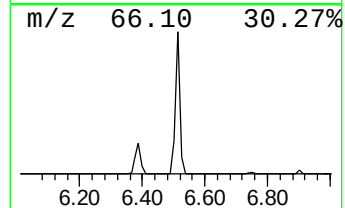
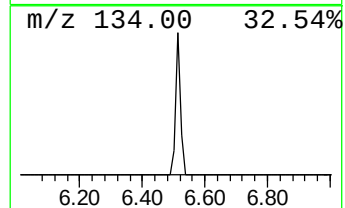
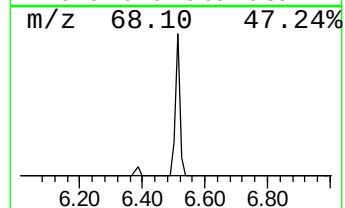
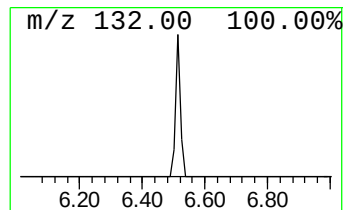
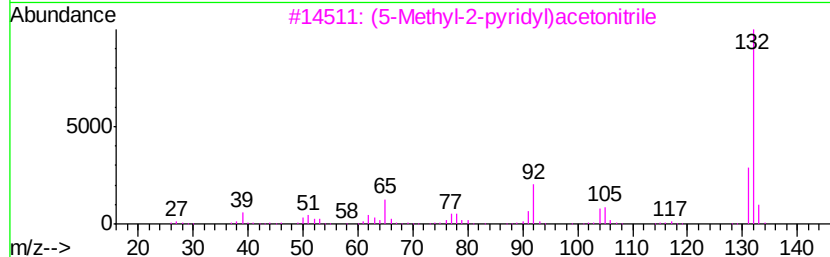
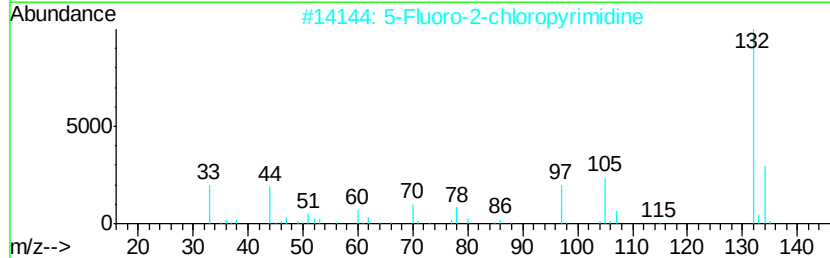
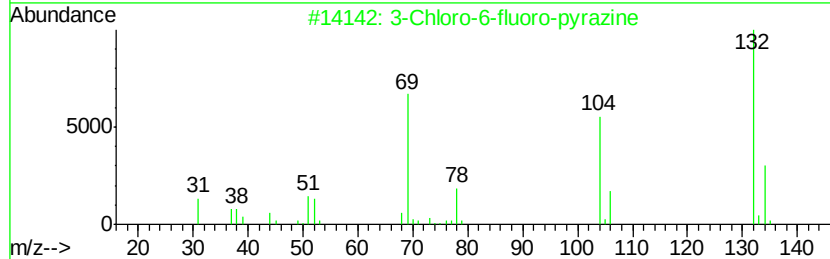
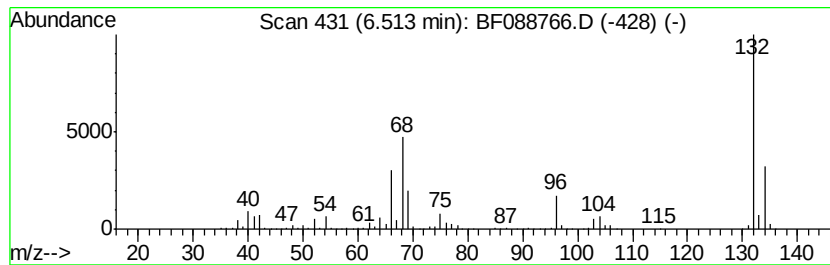
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Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	63.96 ng	1728250	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10	
4	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10	



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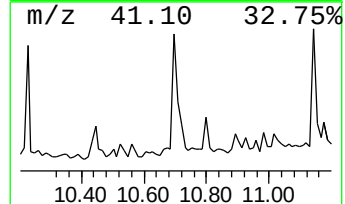
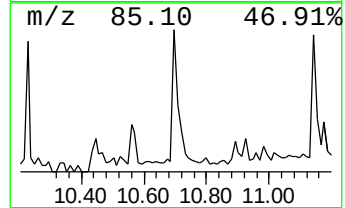
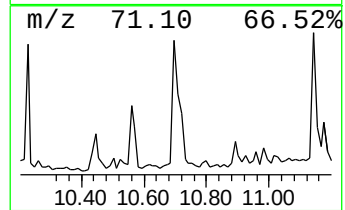
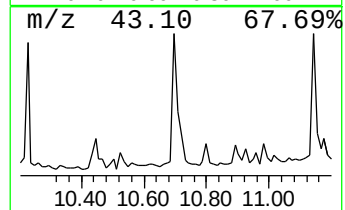
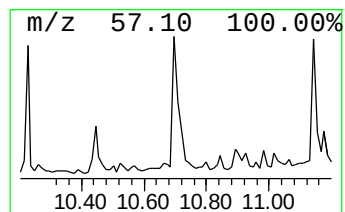
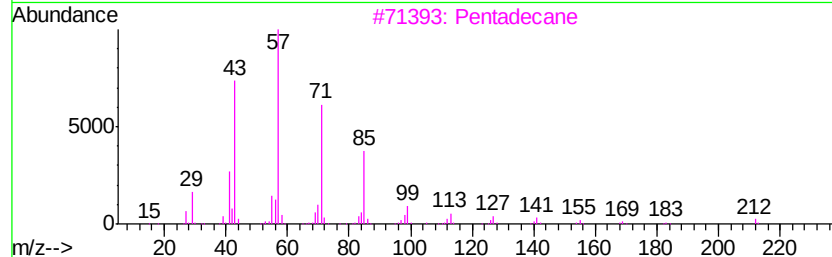
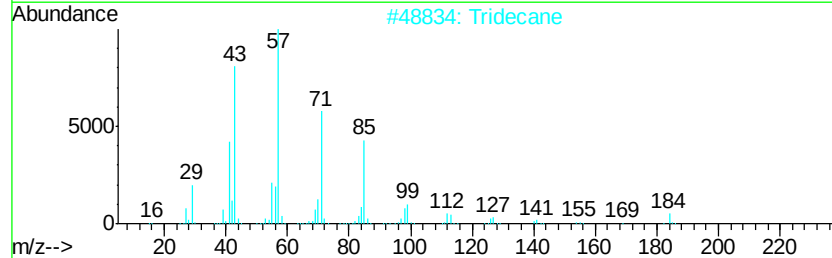
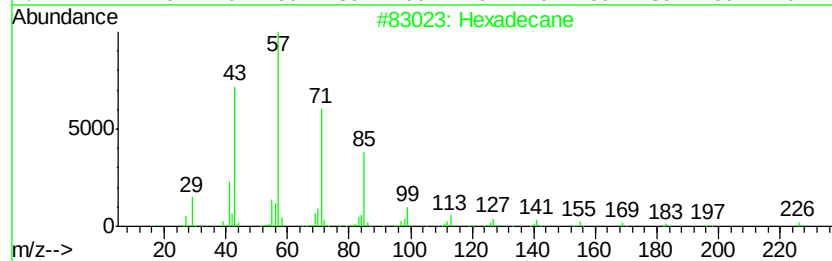
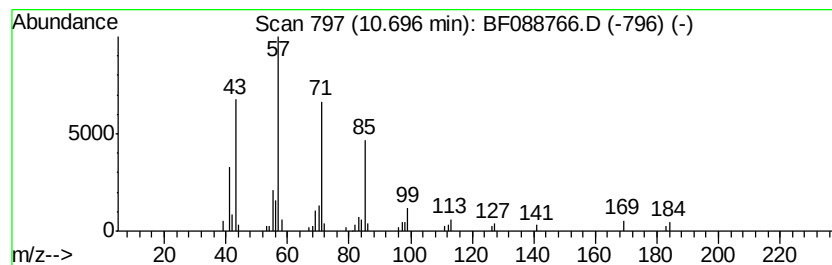
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Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.21 ng	82437	Phenanthrene-d10	11.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Tridecane		184	C13H28	000629-50-5	87
3	Pentadecane		212	C15H32	000629-62-9	86
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
5	Tetradecane		198	C14H30	000629-59-4	86



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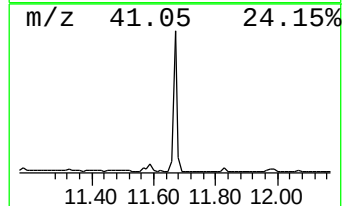
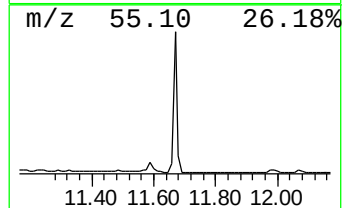
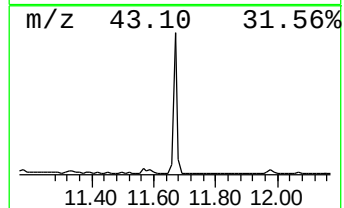
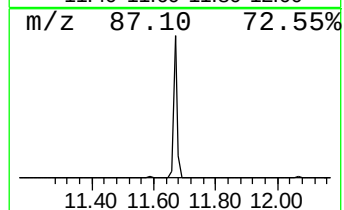
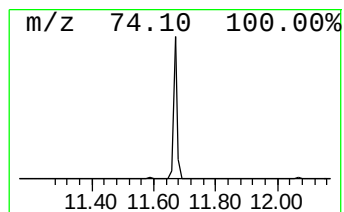
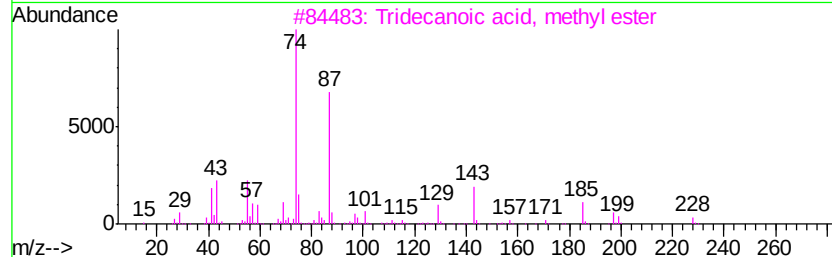
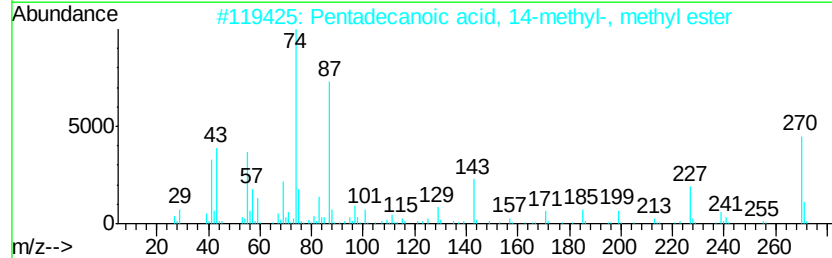
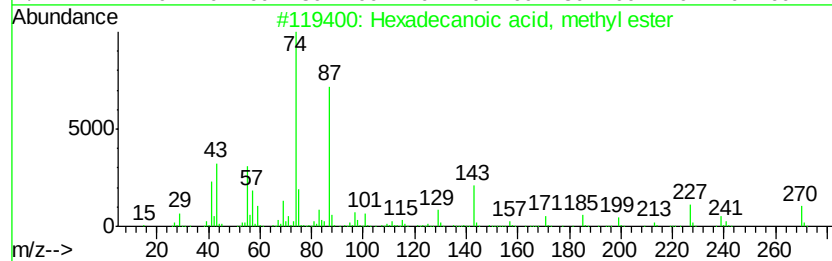
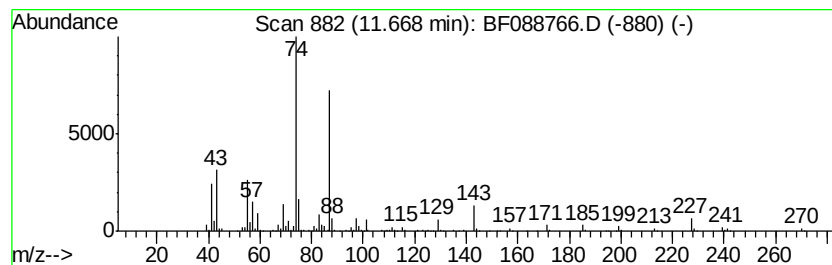
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Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	24.15 ng	898929	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



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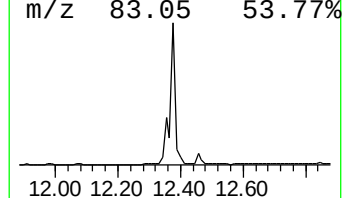
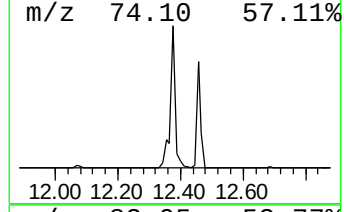
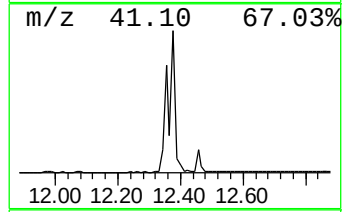
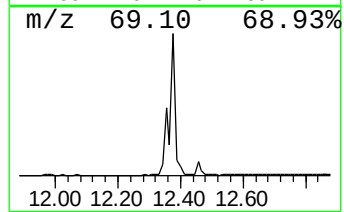
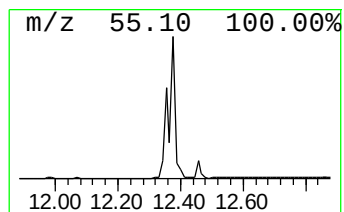
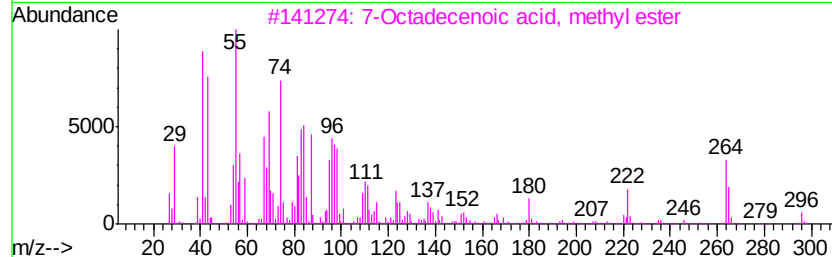
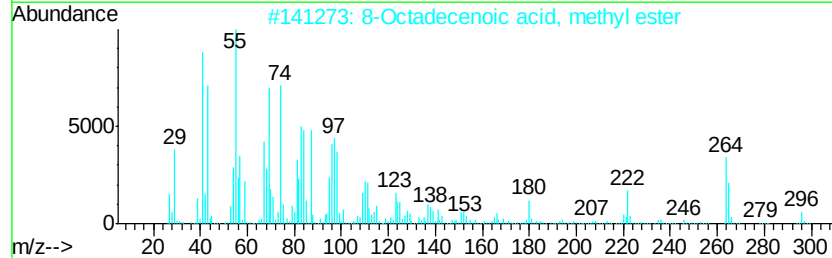
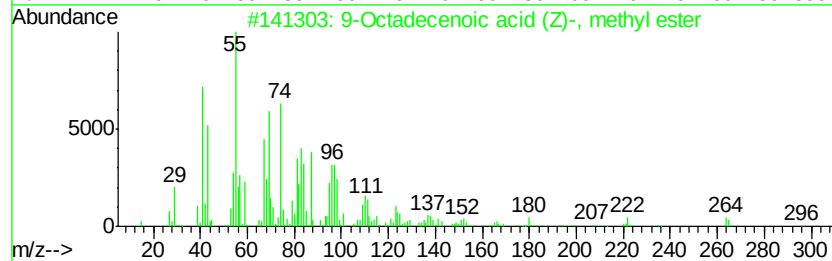
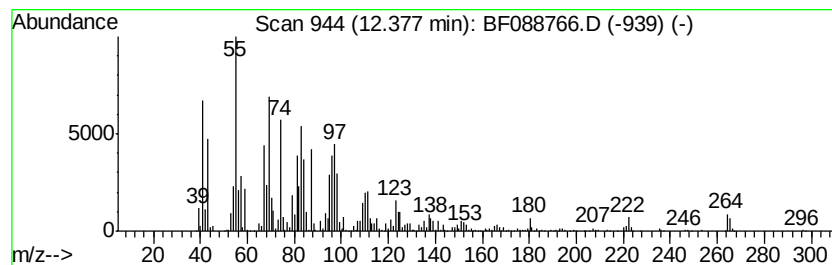
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Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	127.22 ng	4736140	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3		7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
4		6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
5		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91



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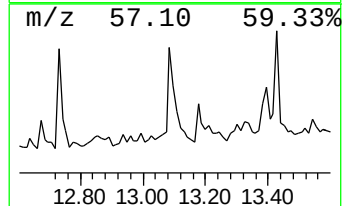
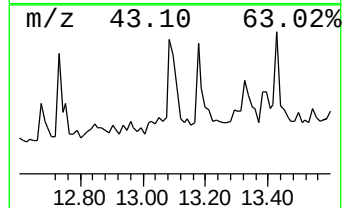
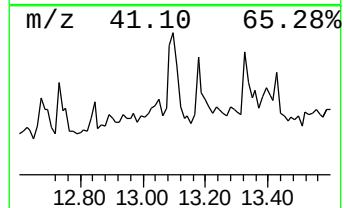
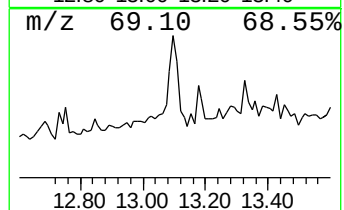
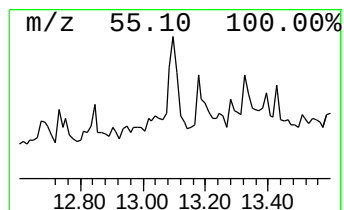
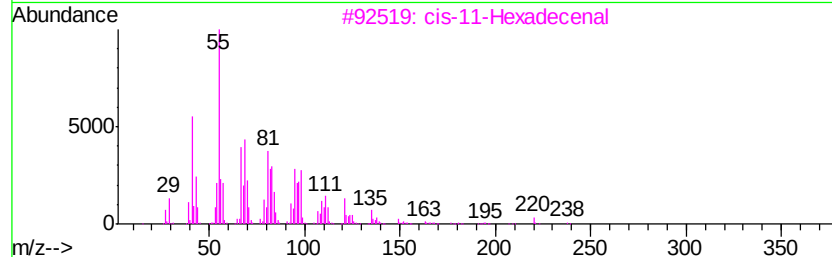
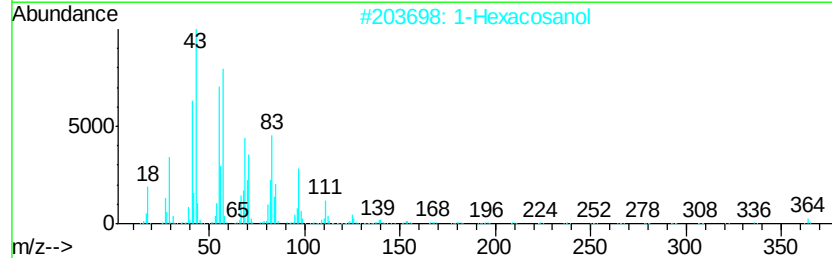
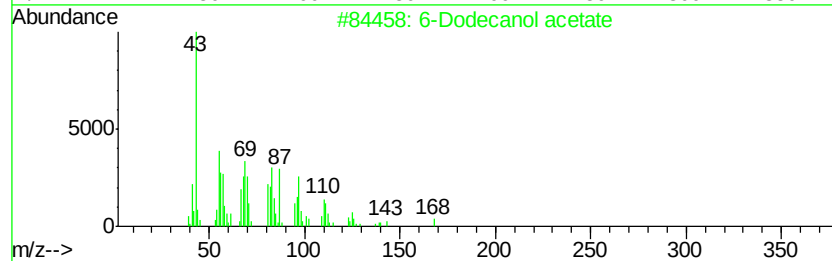
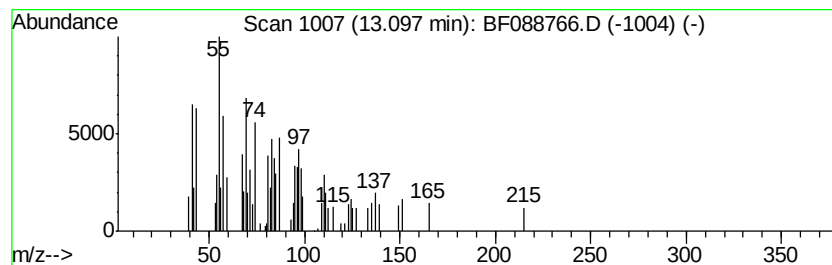
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ClientSampleId :
SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 6-Dodecanol acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.85 ng	91560	Chrysene-d12	13.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	6-Dodecanol acetate	228 C14H28O2	060826-23-5	53
2	1-Hexacosanol	382 C26H54O	000506-52-5	35
3	cis-11-Hexadecenal	238 C16H30O	053939-28-9	35
4	Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8	30
5	1-Eicosanol	298 C20H42O	000629-96-9	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088766.D
Acq On : 7 Jul 2016 6:44
Operator : UM/SJ
Sample : H3870-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

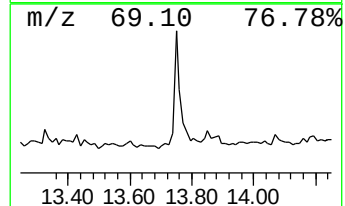
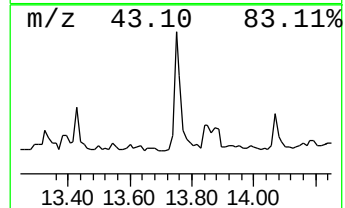
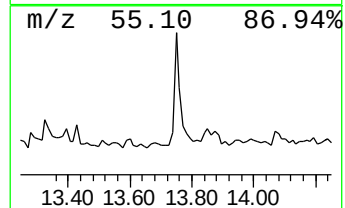
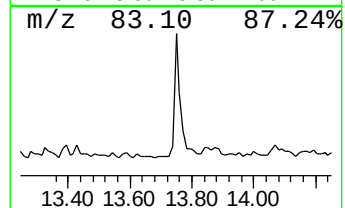
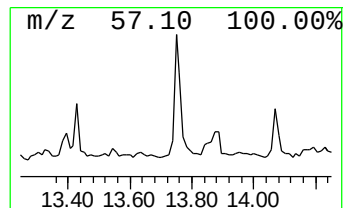
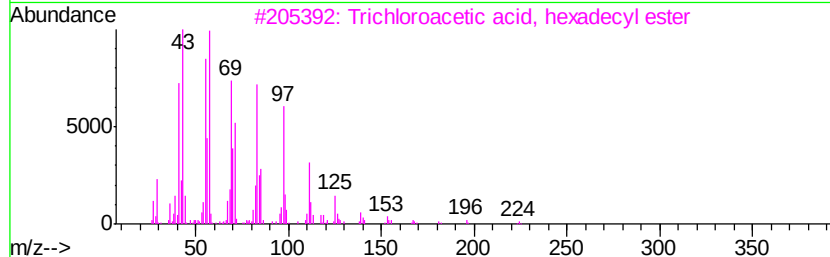
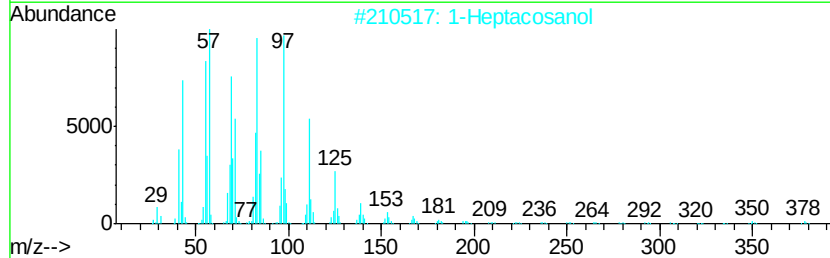
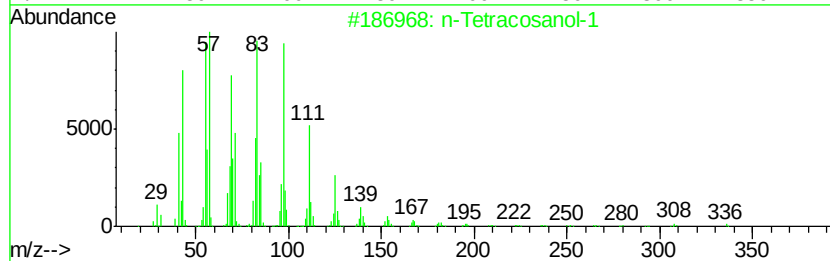
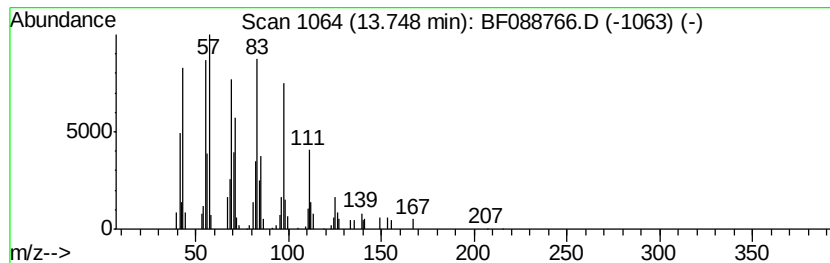
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	3.19 ng	102598	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088766.D
Acq On : 7 Jul 2016 6:44
Operator : UM/SJ
Sample : H3870-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-COMP

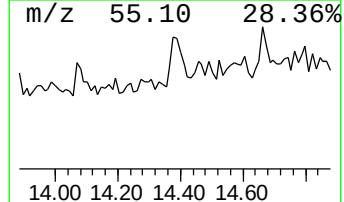
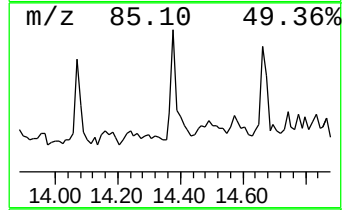
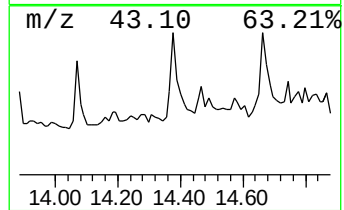
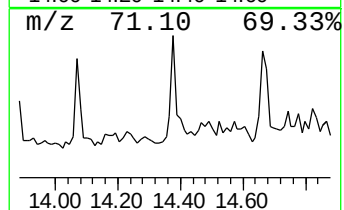
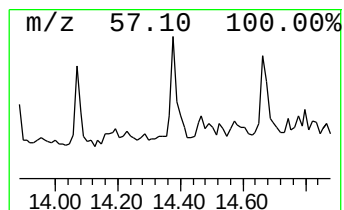
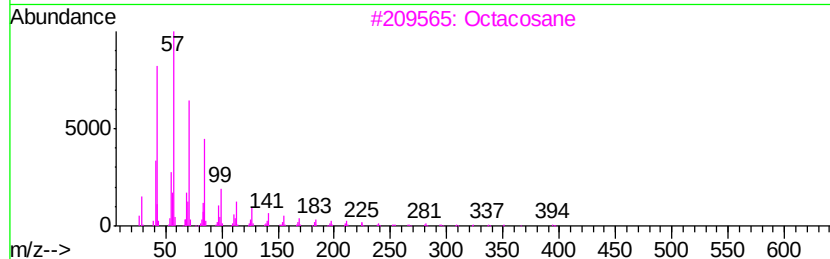
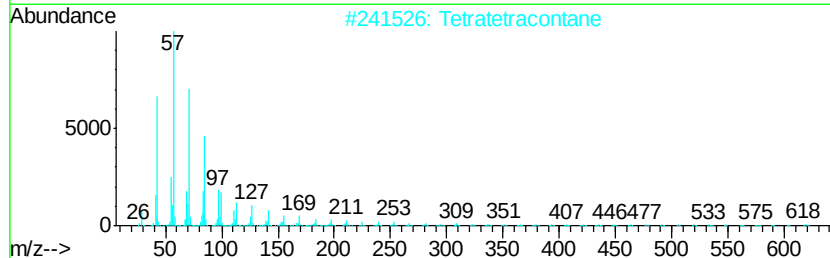
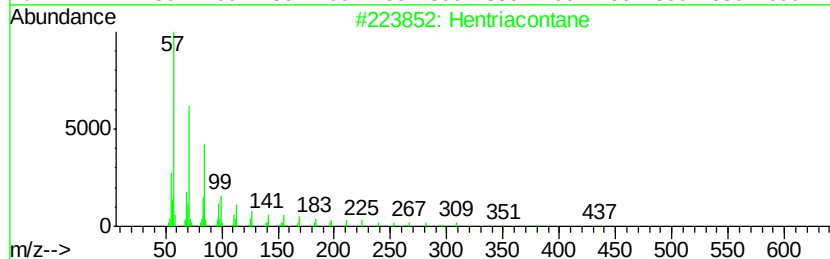
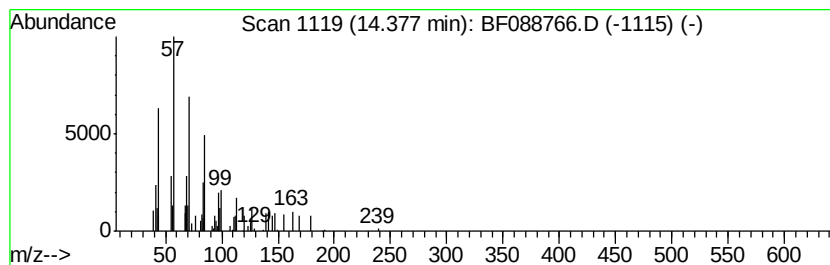
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	2.33 ng	74822	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	74
2		Tetratetracontane	619	C44H90	007098-22-8	72
3		Octacosane	394	C28H58	000630-02-4	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Pentacosane	352	C25H52	000629-99-2	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088766.D
Acq On : 7 Jul 2016 6:44
Operator : UM/SJ
Sample : H3870-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-COMP

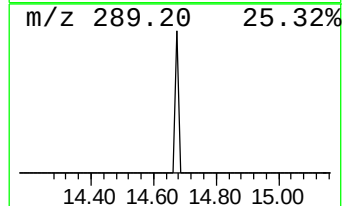
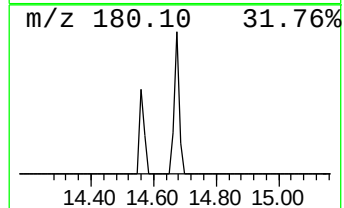
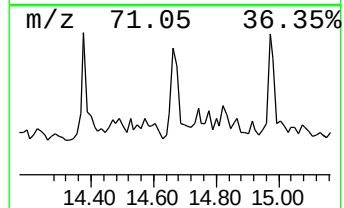
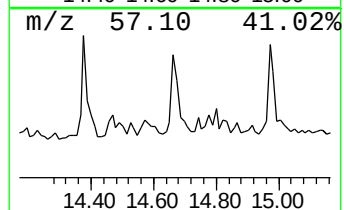
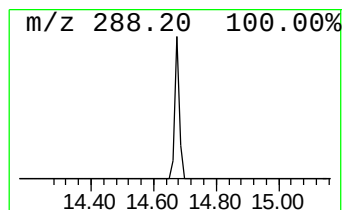
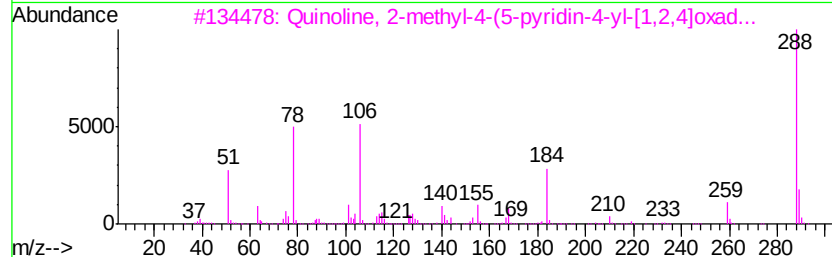
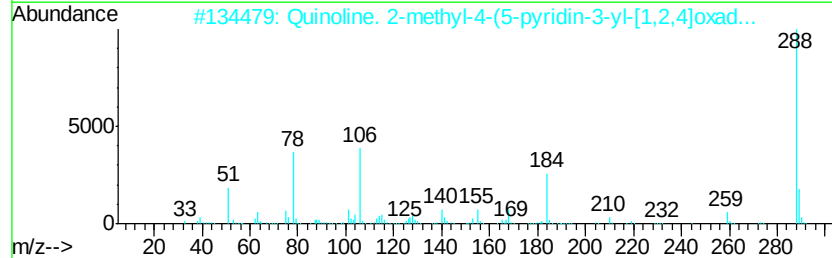
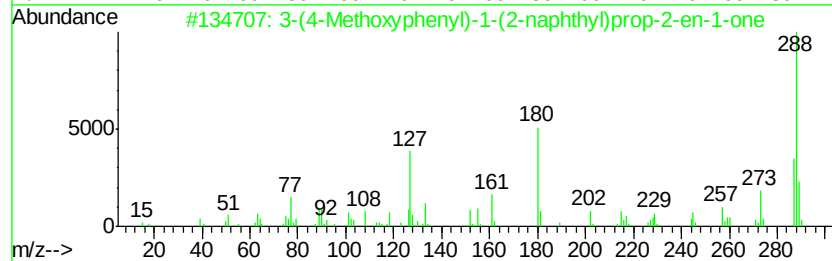
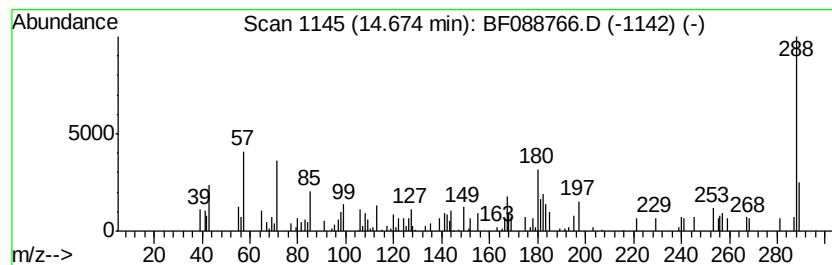
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.67 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.55 ng	64786	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(4-Methoxyphenyl)-1-(2-naphthyl)prop-2-en-1-one	288	C20H16O2	022359-67-7	40
2			Quinoline, 2-methyl-4-(5-pyridin-3-yl[1,2,4]oxadiazol-5-yl)-	288	C17H12N4O	1000317-16-7	38
3			Quinoline, 2-methyl-4-(5-pyridin-3-yl[1,2,4]oxadiazol-5-yl)-	288	C17H12N4O	1000317-16-4	32
4			5-Imidazolic amide, 4-amino-2-[4-(2-methyl-4-(5-pyridin-3-yl[1,2,4]oxadiazol-5-yl)quinolin-2-yl)-5-yl]-	288	C12H12N6O3	1000128-07-1	32
5			2,3,4,5,7a,8,11,12-Octahydro-1H-benzo[1,2-b:4,5-b']dipyrrolo[3,2-a:3',2'-c]quinoline	288	C16H20N2OS	1177856-80-2	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088766.D
Acq On : 7 Jul 2016 6:44
Operator : UM/SJ
Sample : H3870-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.91	5.2	ng	141168	1	6.75	540417	20.0
unknown6.51	6.51	64.0	ng	1728250	1	6.75	540417	20.0
Hexadecane	10.70	2.2	ng	82437	4	11.26	744537	20.0
Hexadecanoic acid...	11.67	24.1	ng	898929	4	11.26	744537	20.0
9-Octadecenoic ac...	12.38	127.2	ng	4736140	4	11.26	744537	20.0
6-Dodecanol acetate	13.10	2.9	ng	91560	5	13.89	643211	20.0
n-Tetracosanol-1	13.75	3.2	ng	102598	5	13.89	643211	20.0
Hentriacontane	14.38	2.3	ng	74822	5	13.89	643211	20.0
unknown14.67	14.67	2.5	ng	64786	6	15.27	507690	20.0