

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051816\
 Data File : BF087160.D
 Acq On : 18 May 2016 23:11
 Operator : UM/SJ
 Sample : H3143-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-I-76(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-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	1.713	9	11	68	rVB	4055338	9080044	100.00%	17.617%
2	4.696	269	272	289	rBV	1506284	2854869	31.44%	5.539%
3	5.164	311	313	316	rBV	3546795	4097617	45.13%	7.950%
4	5.564	346	348	360	rVB	231973	251425	2.77%	0.488%
5	6.250	405	408	410	rBV	4243749	4794035	52.80%	9.302%
6	6.353	414	417	419	rBV	4601813	4770892	52.54%	9.257%
7	6.582	434	437	439	rBV	604483	897915	9.89%	1.742%
8	6.730	448	450	453	rBV	3352834	3061626	33.72%	5.940%
9	7.153	484	487	489	rBV	3010541	3011133	33.16%	5.842%
10	7.862	547	549	552	rBV	1276678	1188271	13.09%	2.306%
11	8.948	641	644	646	rBV	3933471	4308816	47.45%	8.360%
12	9.348	677	679	681	rBV	569036	537393	5.92%	1.043%
13	9.553	696	697	699	rBV	111975	117086	1.29%	0.227%
14	9.610	699	702	704	rBV	1534413	1350661	14.88%	2.621%
15	10.056	738	741	742	rBV	215564	183361	2.02%	0.356%
16	10.273	757	760	763	rBV	70090	106469	1.17%	0.207%
17	10.399	768	771	774	rBV	2805995	2932583	32.30%	5.690%
18	10.525	780	782	786	rBV	247362	306670	3.38%	0.595%
19	10.662	792	794	797	rVB3	52230	106386	1.17%	0.206%
20	10.719	797	799	802	rBV2	48741	99682	1.10%	0.193%
21	10.811	805	807	809	rVV	69231	98219	1.08%	0.191%
22	11.085	829	831	835	rVB	1450223	1278513	14.08%	2.481%
23	11.634	877	879	884	rBV	85263	116546	1.28%	0.226%
24	12.674	967	970	972	rBV	2925786	3327818	36.65%	6.457%
25	13.599	1047	1051	1058	rBV	93857	303584	3.34%	0.589%
26	13.714	1058	1061	1063	rBV	923564	1004181	11.06%	1.948%
27	14.240	1104	1107	1110	rBV3	43829	126282	1.39%	0.245%
28	14.548	1132	1134	1137	rBV	108313	121673	1.34%	0.236%
29	15.062	1177	1179	1182	rBV	784003	884307	9.74%	1.716%
30	15.451	1211	1213	1219	rBV2	48949	118504	1.31%	0.230%
31	15.623	1226	1228	1232	rVB3	55307	103599	1.14%	0.201%

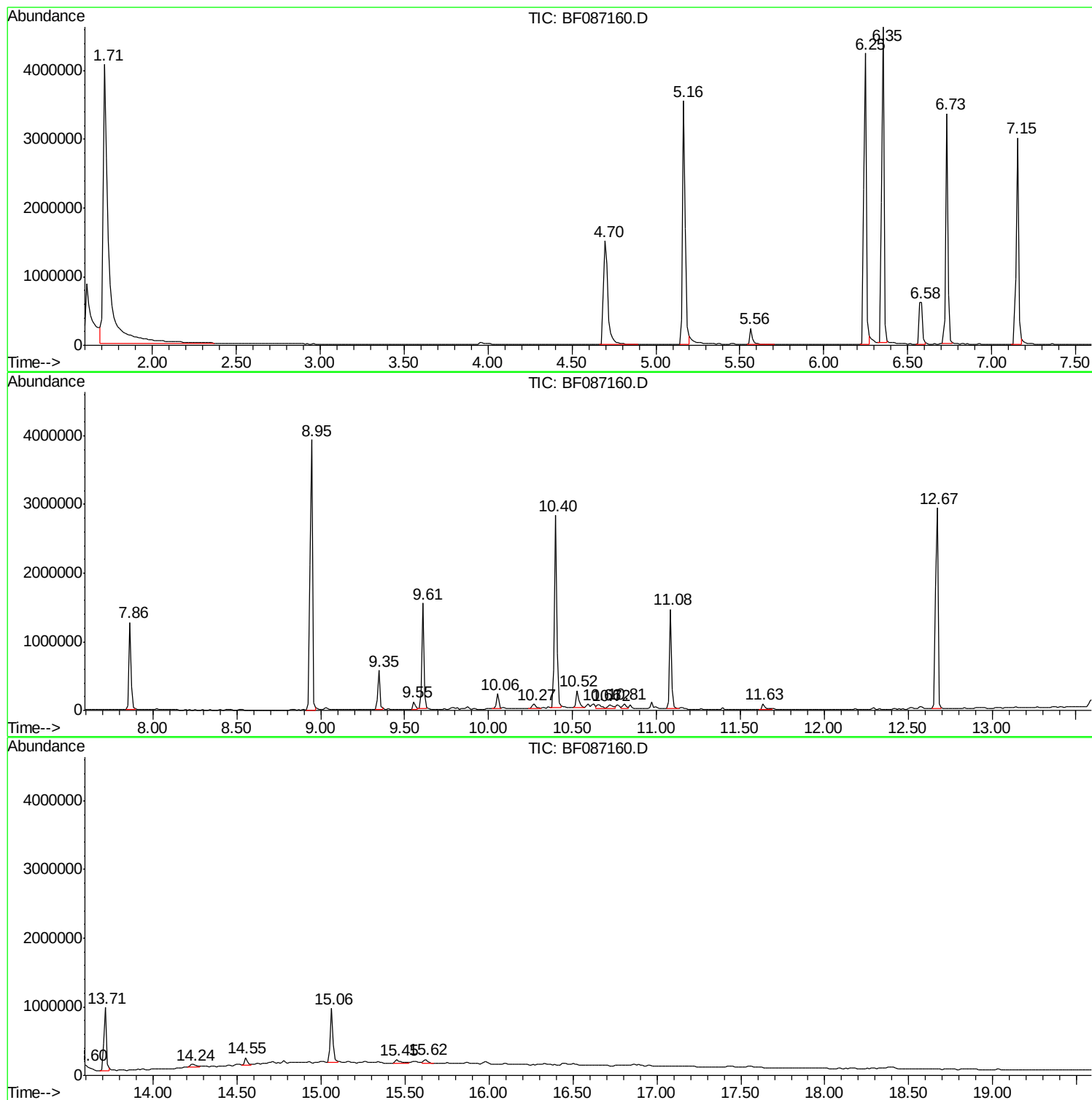
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Instrument :
BNA_F
ClientSampleId :
2-I-76(0-2)

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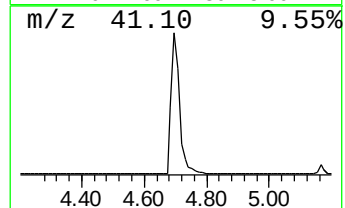
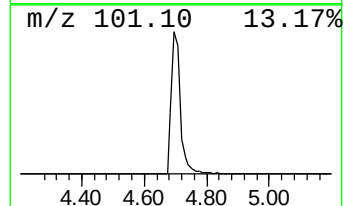
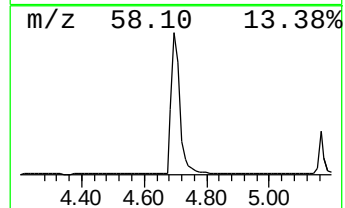
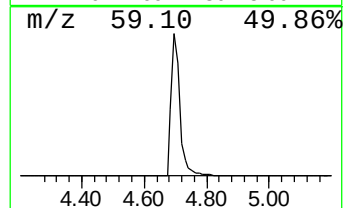
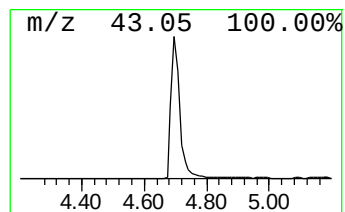
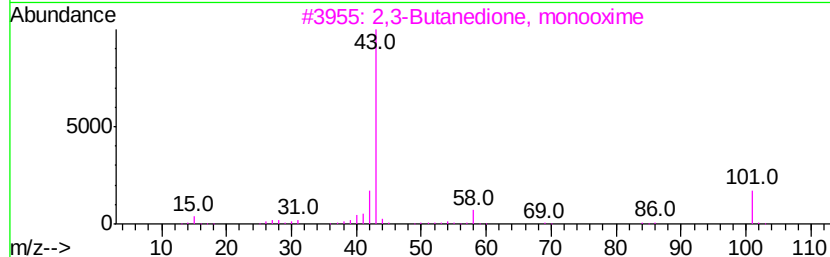
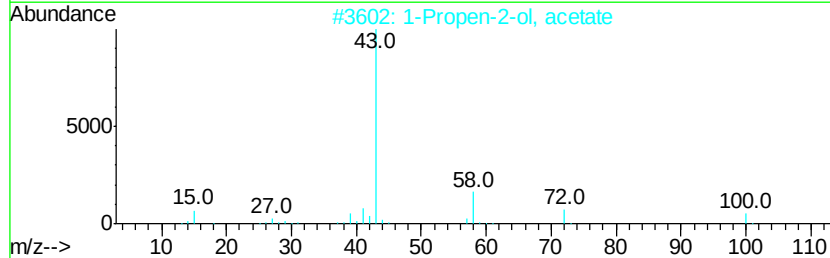
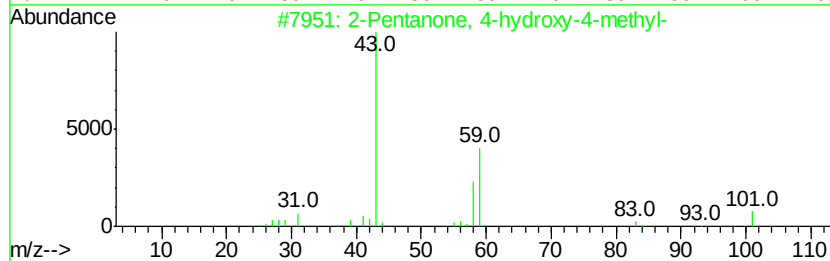
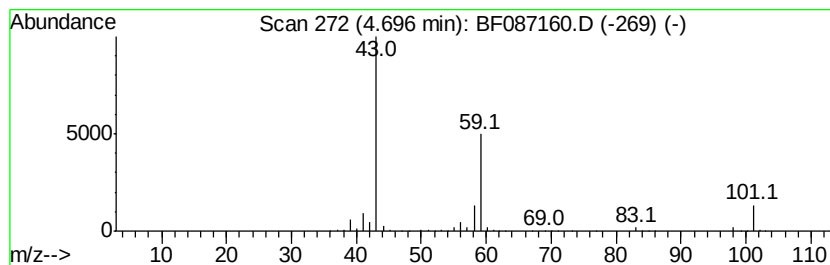
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.70	63.59 ng	2854870	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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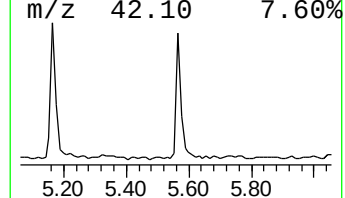
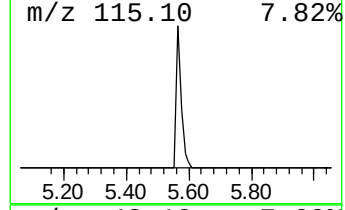
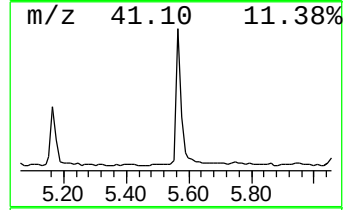
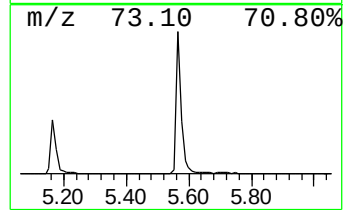
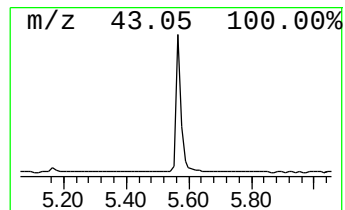
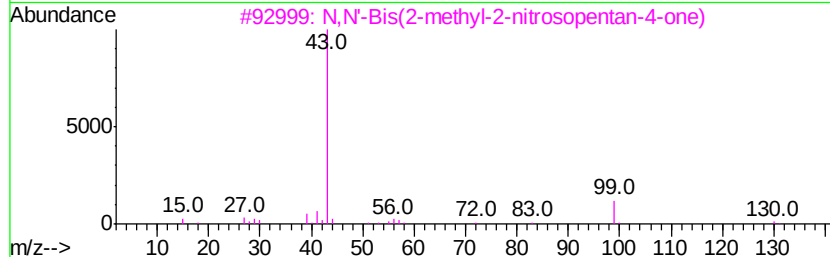
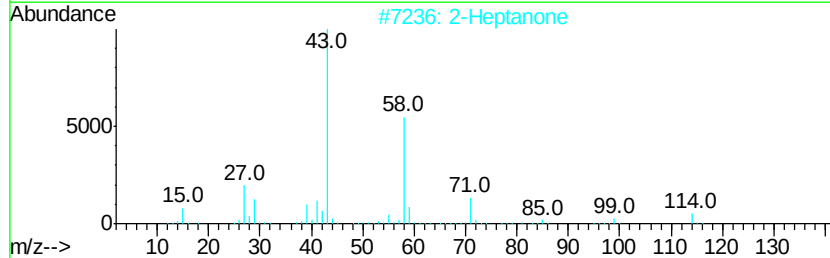
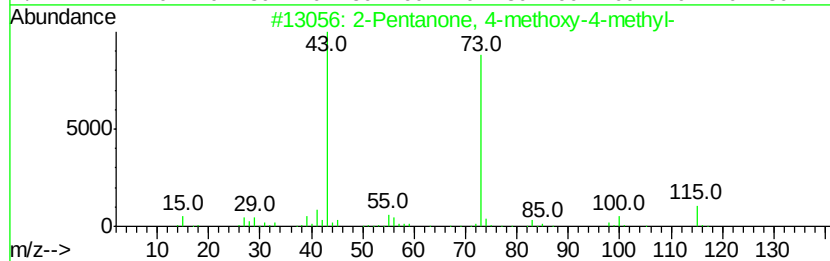
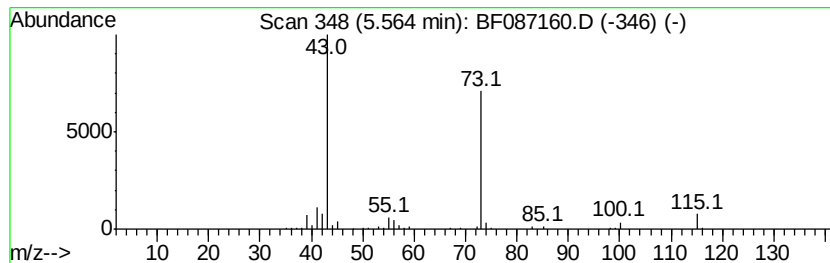
Instrument :
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2-I-76(0-2)

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 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.56	5.60 ng	251425	1,4-Dichlorobenzene-d4	6.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	2-Heptanone	114	C7H14O	000110-43-0	23
3	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	23
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12
5	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	12



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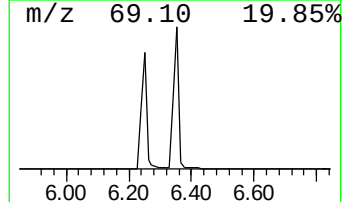
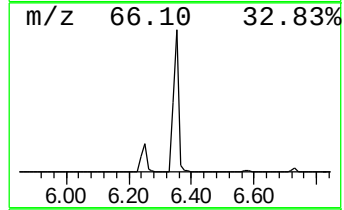
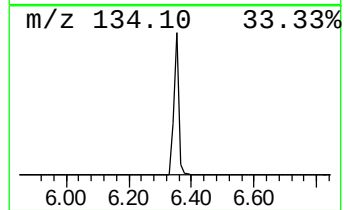
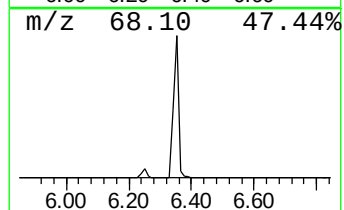
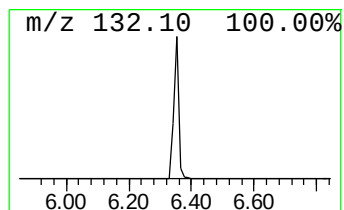
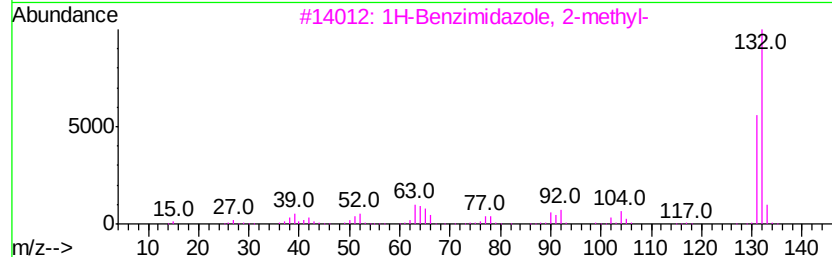
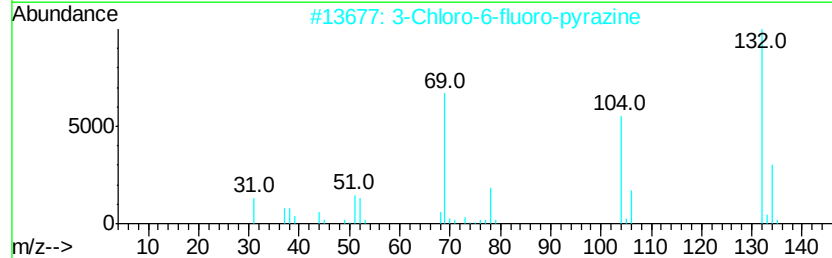
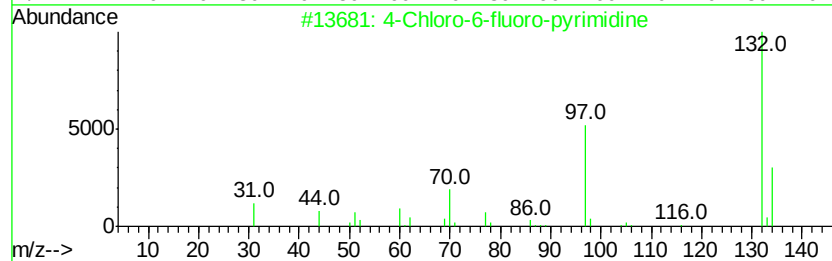
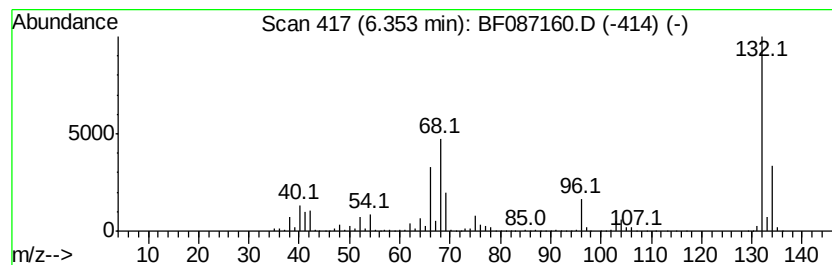
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	106.27 ng	4770890	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	12



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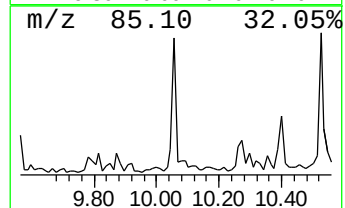
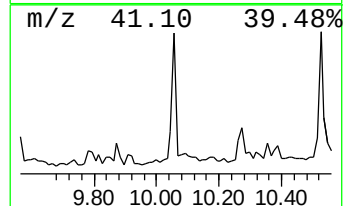
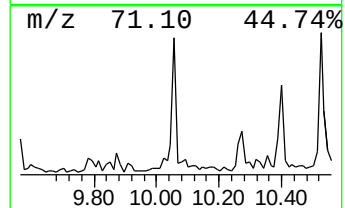
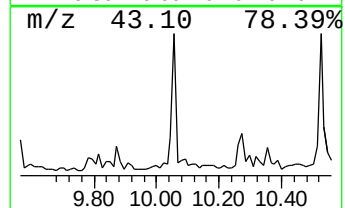
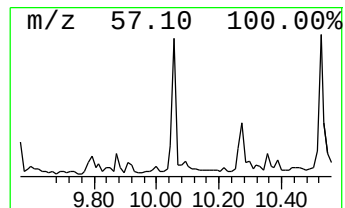
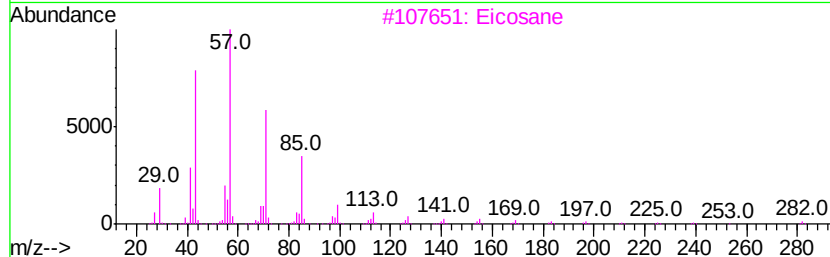
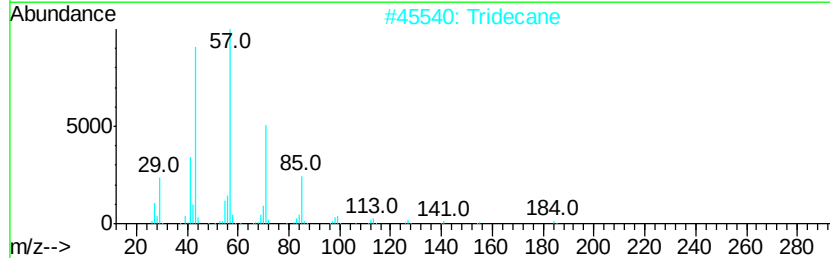
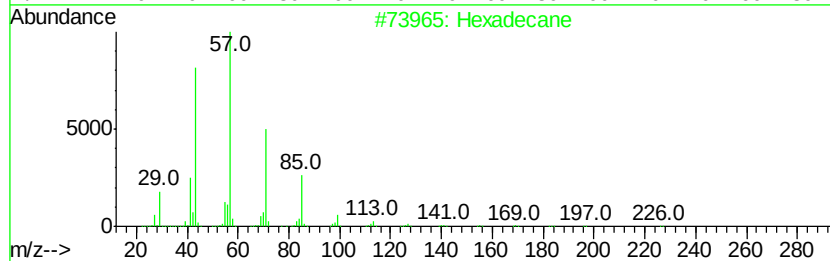
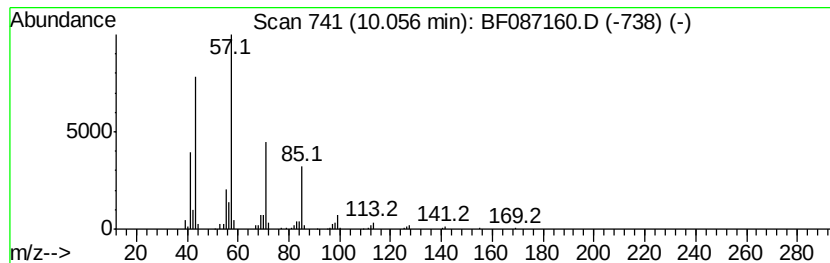
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	2.72 ng	183361	Acenaphthene-d10	9.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Eicosane		282	C20H42	000112-95-8	86
4	Octadecane		254	C18H38	000593-45-3	80
5	Tetradecane		198	C14H30	000629-59-4	72



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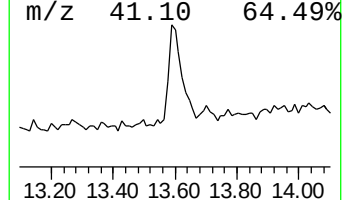
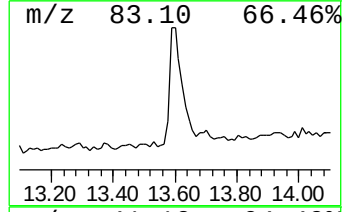
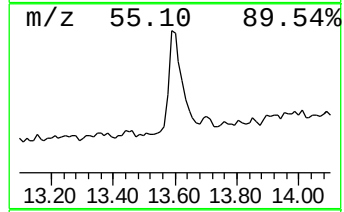
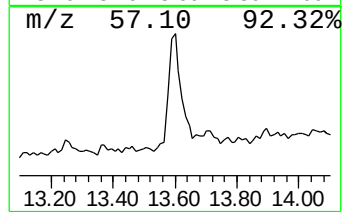
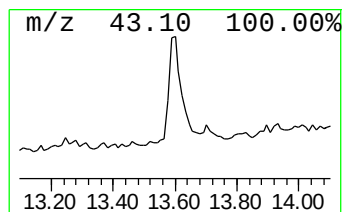
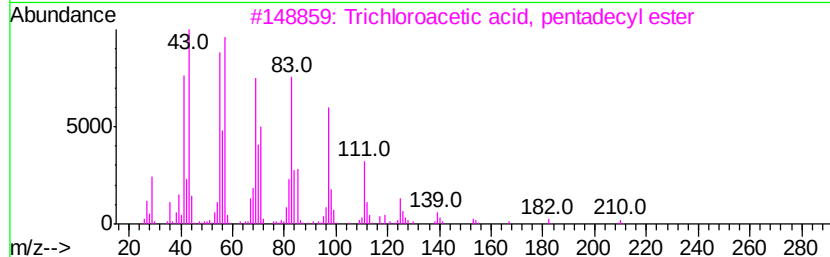
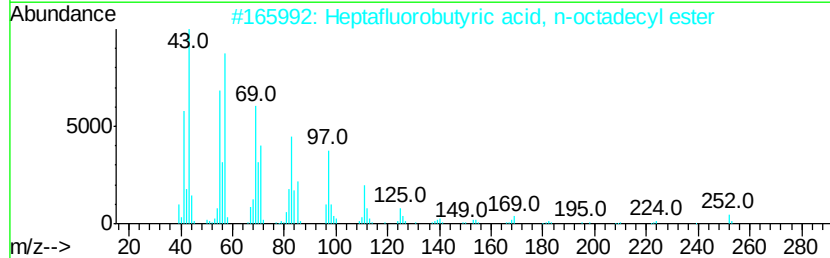
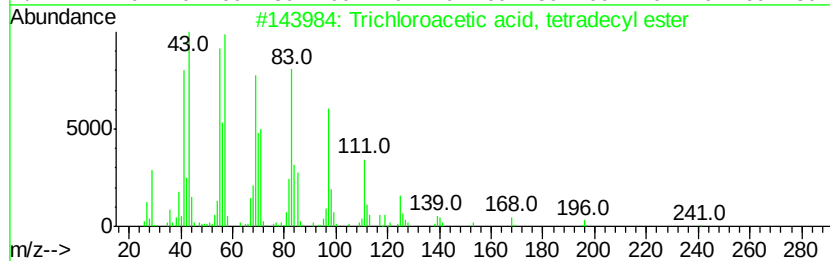
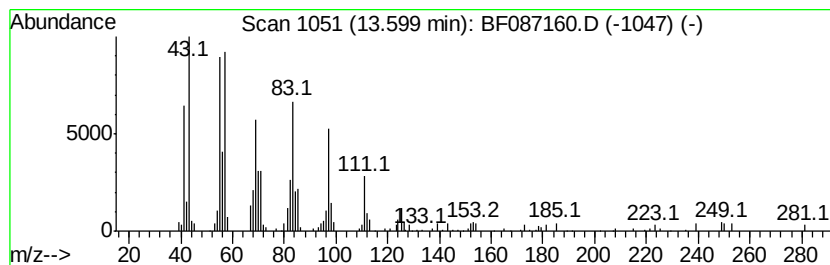
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trichloroacetic acid, tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	6.05 ng	303584	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		1,2-Octadecanediol	286	C18H38O2	020294-76-2	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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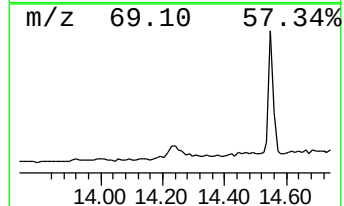
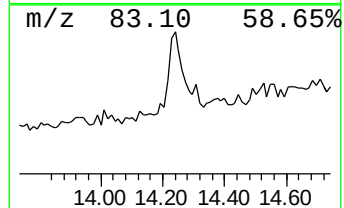
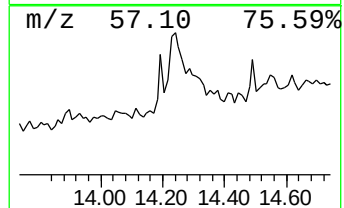
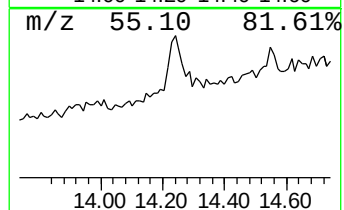
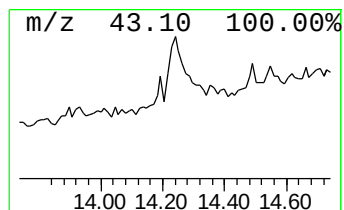
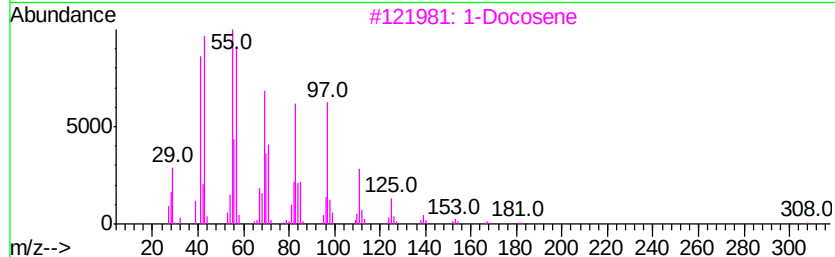
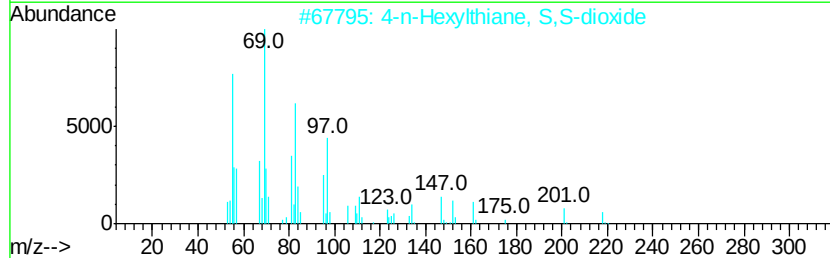
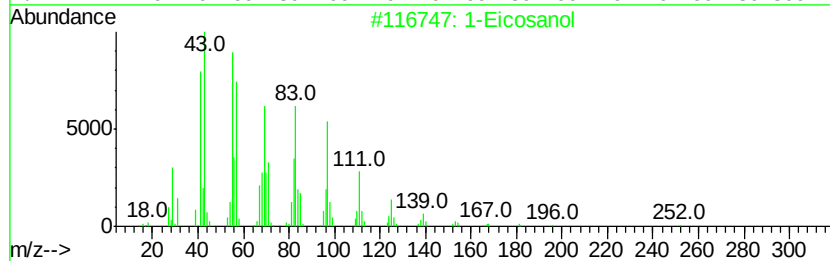
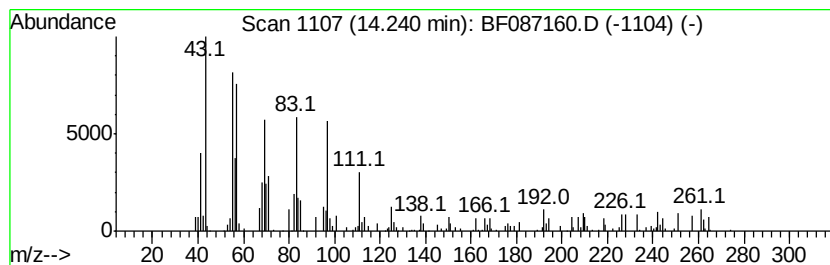
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Eicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.52 ng	126282	Chrysene-d12	13.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	64
2	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	49
3	1-Docosene	308	C22H44	001599-67-3	46
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	43
5	Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-95-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051816\
Data File : BF087160.D
Acq On : 18 May 2016 23:11
Operator : UM/SJ
Sample : H3143-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-I-76(0-2)

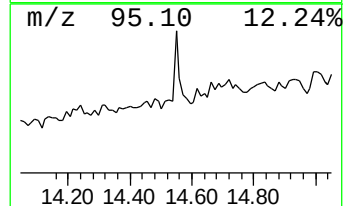
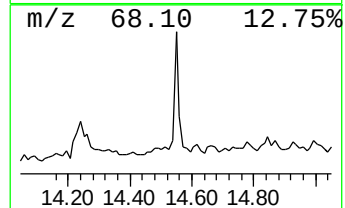
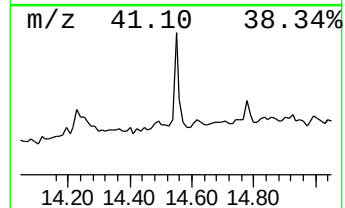
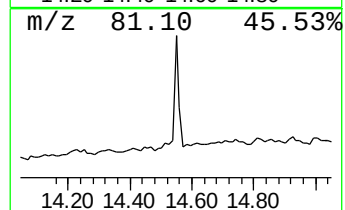
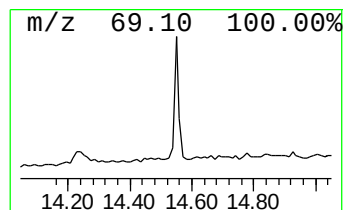
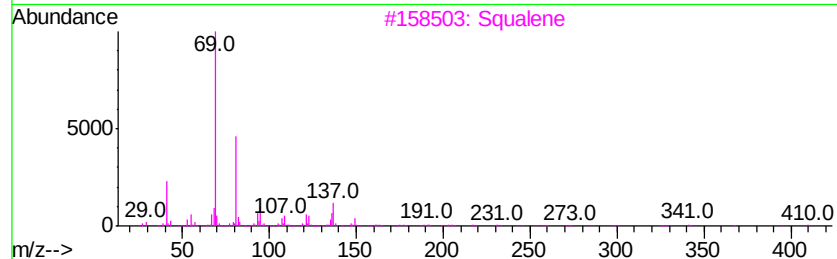
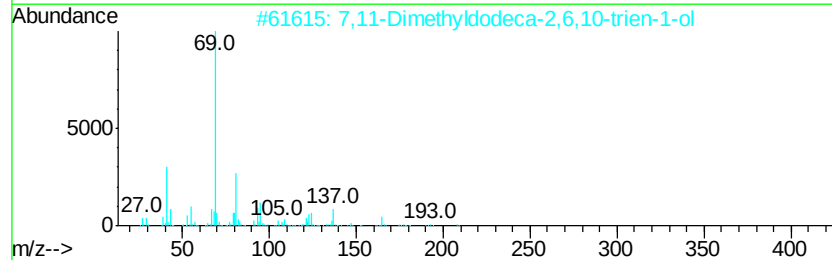
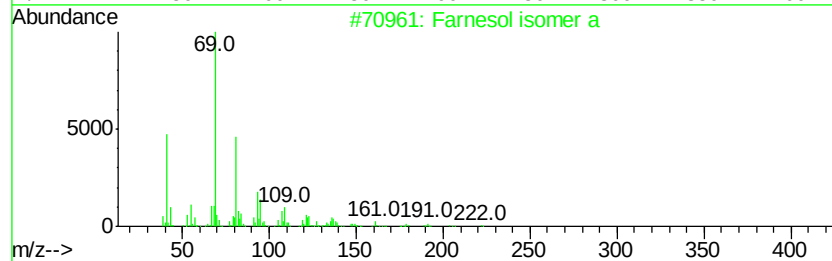
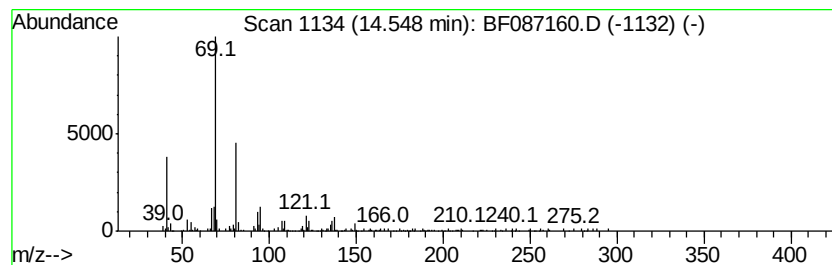
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Farnesol isomer a Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.75 ng	121673	Perylene-d12	15.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a		222	C15H26O	1000108-92-4	81
2	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	74
3	Squalene		410	C30H50	007683-64-9	74
4	4-Methyl-1,5-Heptadiene		110	C8H14	000998-94-7	72
5	2,6-Octadiene, 2,6-dimethyl-		138	C10H18	002792-39-4	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051816\
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Acq On : 18 May 2016 23:11
Operator : UM/SJ
Sample : H3143-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

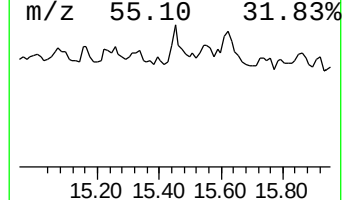
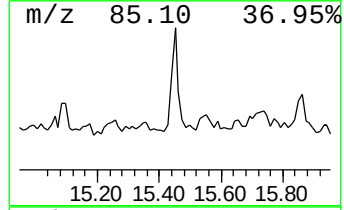
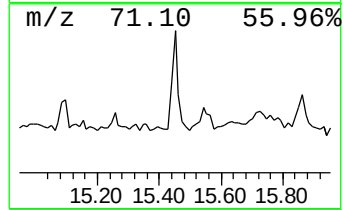
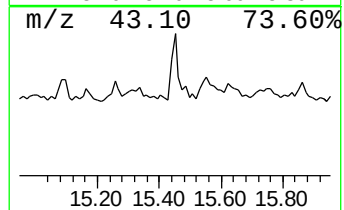
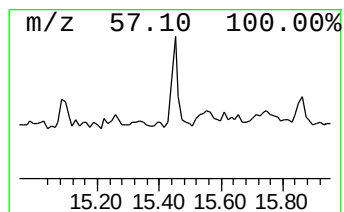
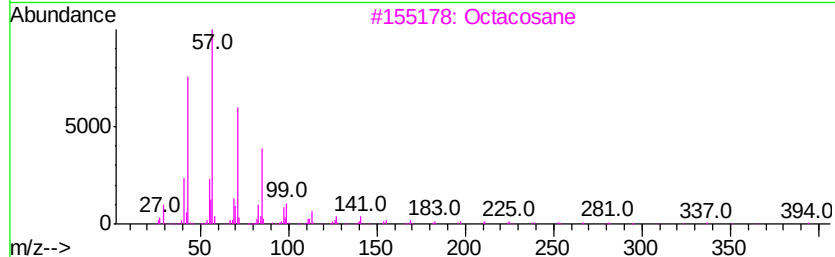
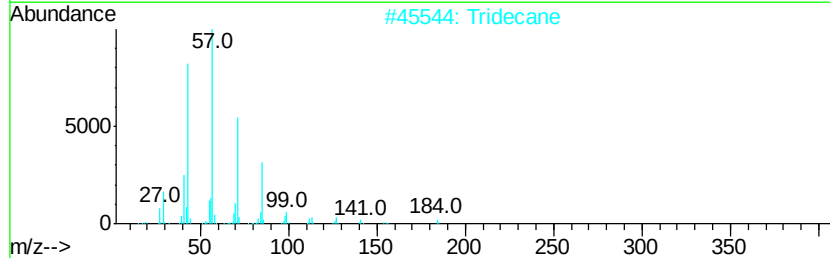
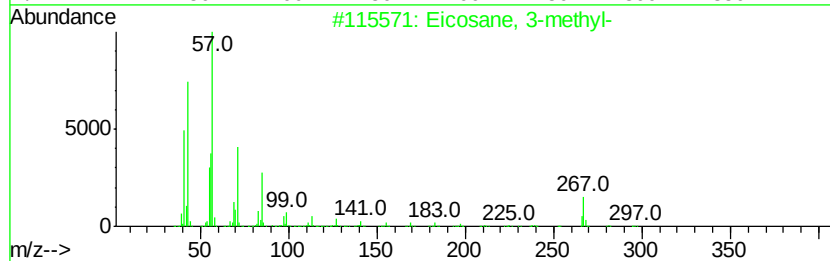
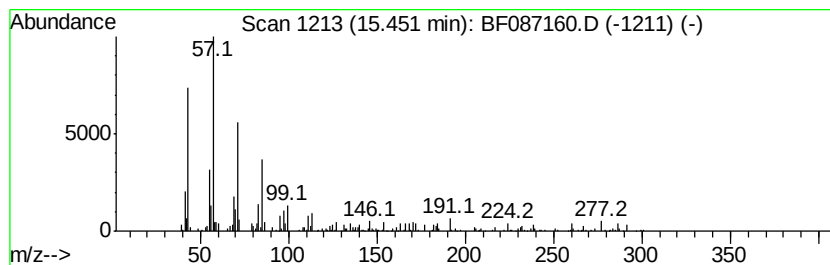
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.68 ng	118504	Perylene-d12	15.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane, 3-methyl-	296 C21H44	006418-46-8	60
2	Tridecane	184 C13H28	000629-50-5	58
3	Octacosane	394 C28H58	000630-02-4	53
4	Dodecane	170 C12H26	000112-40-3	53
5	Hexatriacontane	507 C36H74	000630-06-8	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051816\
Data File : BF087160.D
Acq On : 18 May 2016 23:11
Operator : UM/SJ
Sample : H3143-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

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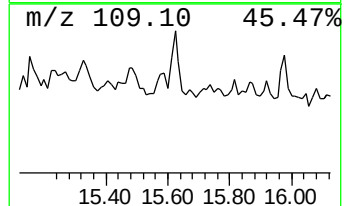
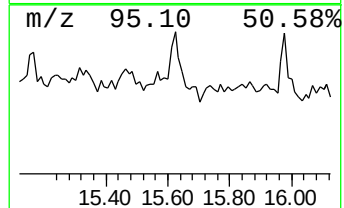
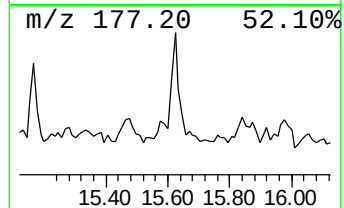
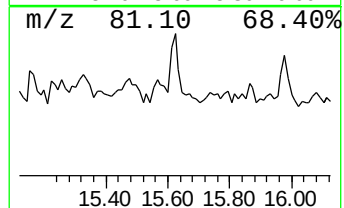
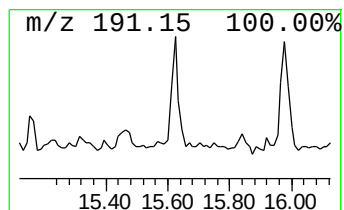
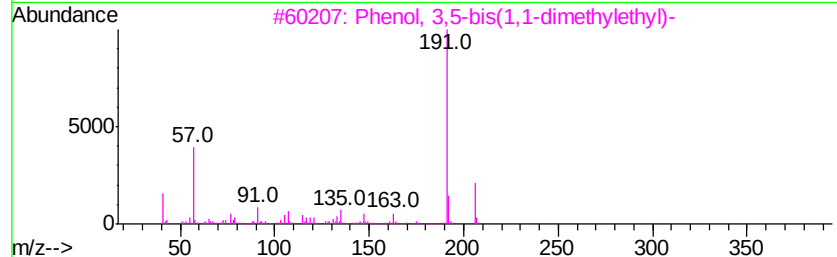
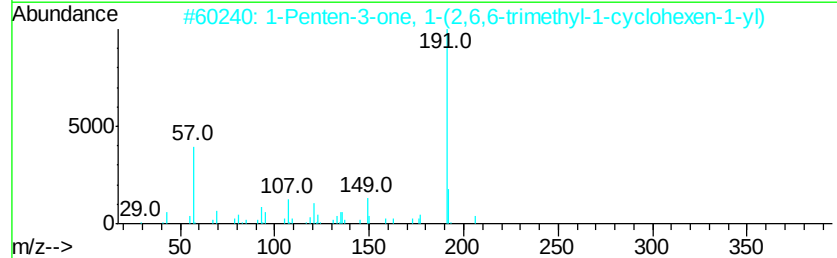
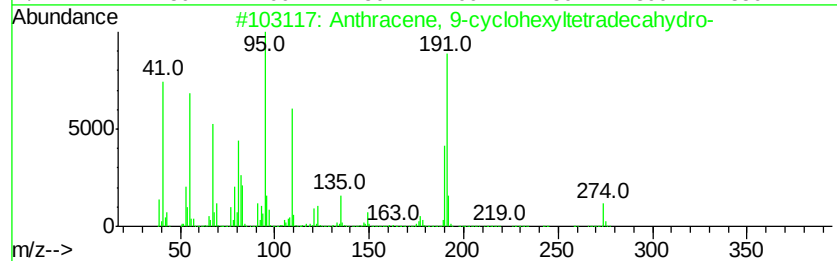
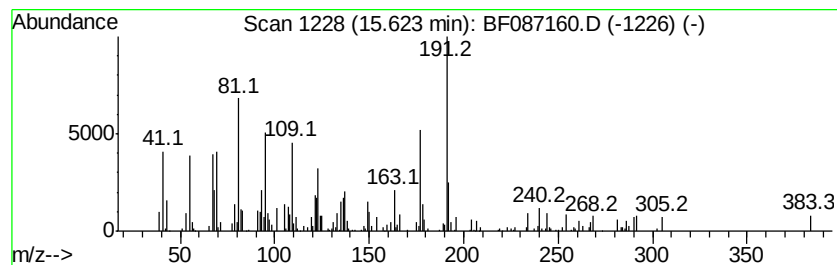
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.62 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.34 ng	103599	Perylene-d12	15.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	35
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	22
3		Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	22
4		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	14
5		Protriptyline, N-acetyl-	305	C21H23NO	023047-28-1	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051816\
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Sample : H3143-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-I-76(0-2)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	63.6	ng	2854870	1	6.58	897915	20.0
2-Pentanone, 4-me...	5.56	5.6	ng	251425	1	6.58	897915	20.0
unknown6.35	6.35	106.3	ng	4770890	1	6.58	897915	20.0
Hexadecane	10.06	2.7	ng	183361	3	9.61	1350660	20.0
Trichloroacetic a...	13.60	6.0	ng	303584	5	13.71	1004180	20.0
1-Eicosanol	14.24	2.5	ng	126282	5	13.71	1004180	20.0
Farnesol isomer a	14.55	2.8	ng	121673	6	15.06	884307	20.0
Eicosane, 3-methyl-	15.45	2.7	ng	118504	6	15.06	884307	20.0
unknown15.62	15.62	2.3	ng	103599	6	15.06	884307	20.0