

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
 Data File : BF088613.D
 Acq On : 2 Jul 2016 13:16
 Operator : UM/SJ
 Sample : H3871-11
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K8-B2(0-11)C

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	1.724	11	12	22	rVB	126765	201779	7.59%	0.805%
2	1.861	22	24	36	rVB	622342	1266044	47.65%	5.051%
3	3.004	123	124	133	rBV3	24766	48054	1.81%	0.192%
4	4.959	292	295	299	rBV	147564	194652	7.33%	0.777%
5	5.393	330	333	335	rBV	1913440	2499484	94.07%	9.972%
6	6.433	421	424	426	rBV	1968738	2657084	100.00%	10.600%
7	6.559	432	435	437	rBV	2533425	2346583	88.31%	9.362%
8	6.787	453	455	458	rBV	577034	629300	23.68%	2.511%
9	6.947	467	469	472	rVB	2048684	1822869	68.60%	7.272%
10	7.359	502	505	507	rBV	1706558	1799592	67.73%	7.179%
11	8.079	565	568	570	rBV	1025797	893922	33.64%	3.566%
12	9.153	660	662	665	rVB	2481218	2481165	93.38%	9.899%
13	9.428	684	686	689	rBV	59631	71434	2.69%	0.285%
14	9.553	694	697	699	rVB	242510	289860	10.91%	1.156%
15	9.770	715	716	719	rBV	34892	29672	1.12%	0.118%
16	9.828	719	721	724	rVB	1090473	921271	34.67%	3.675%
17	10.273	758	760	761	rVB	52737	39981	1.50%	0.160%
18	10.616	787	790	792	rBV	1292700	1470828	55.35%	5.868%
19	10.742	800	801	803	rBV	55591	55020	2.07%	0.220%
20	11.188	838	840	842	rBV	95895	87025	3.28%	0.347%
21	11.302	848	850	852	rVB	894749	792884	29.84%	3.163%
22	11.371	852	856	860	rVB3	17321	43687	1.64%	0.174%
23	11.542	869	871	876	rVV	104452	113994	4.29%	0.455%
24	11.611	876	877	880	rVB	29548	33867	1.27%	0.135%
25	11.839	895	897	899	rBV	84464	102128	3.84%	0.407%
26	12.628	963	966	971	rBV	127431	159809	6.01%	0.638%
27	12.891	986	989	991	rBV	2117828	1894449	71.30%	7.558%
28	13.245	1016	1020	1022	rBV	31016	68240	2.57%	0.272%
29	13.359	1027	1030	1032	rVV2	31752	74420	2.80%	0.297%
30	13.794	1065	1068	1073	rBV3	118673	262132	9.87%	1.046%
31	13.931	1077	1080	1082	rVV	704658	711328	26.77%	2.838%
32	13.977	1082	1084	1089	rVB	47898	140816	5.30%	0.562%
33	14.114	1094	1096	1099	rBV	26567	44195	1.66%	0.176%
34	14.422	1121	1123	1125	rBV	34690	37652	1.42%	0.150%

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ClientSampleId :
K8-B2(0-11)C

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

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35	14.719	1147	1149	1153	rVV	23973	32343	1.22%	0.129%
36	14.788	1153	1155	1157	rVB	56778	58566	2.20%	0.234%
37	15.028	1174	1176	1179	rVB	31577	47846	1.80%	0.191%
38	15.325	1199	1202	1205	rBV	527872	611663	23.02%	2.440%
39	15.382	1205	1207	1209	rBV2	16994	30338	1.14%	0.121%

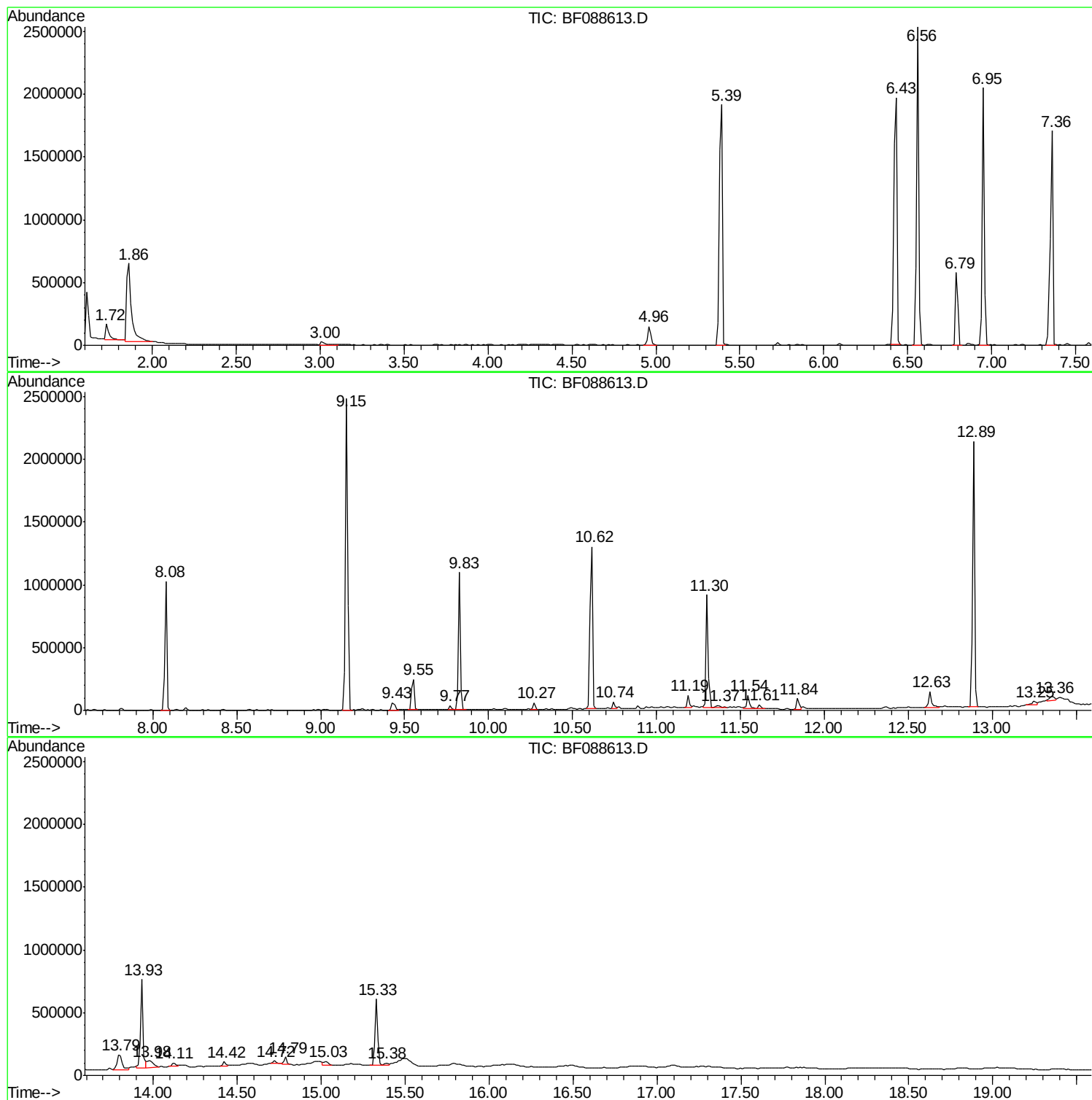
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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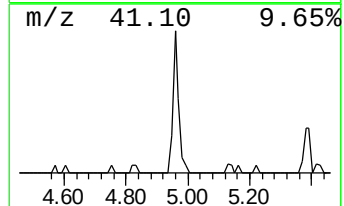
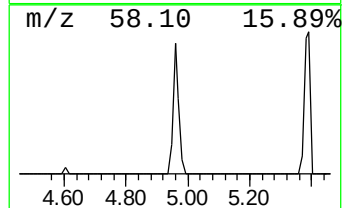
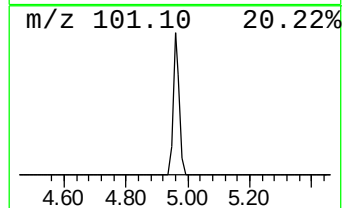
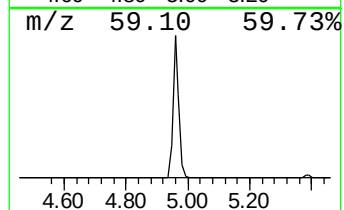
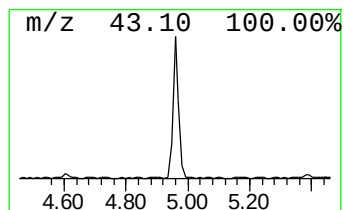
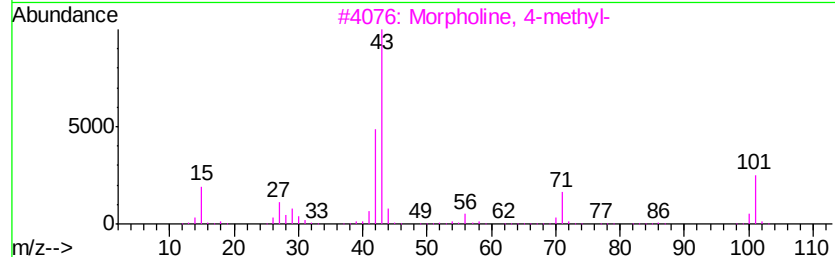
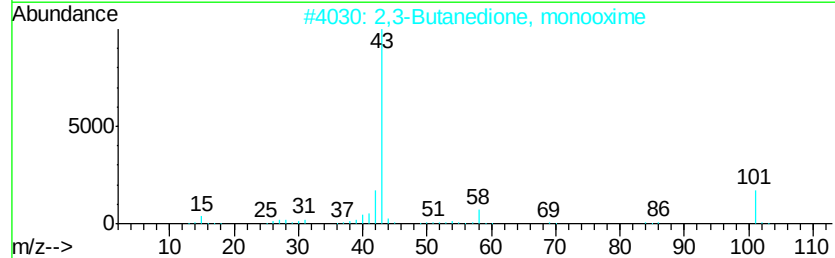
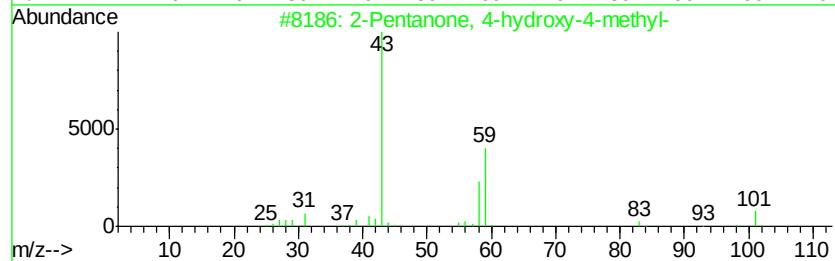
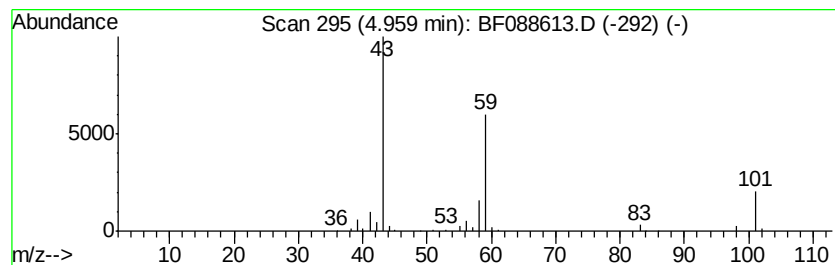
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown4.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	6.19 ng	194652	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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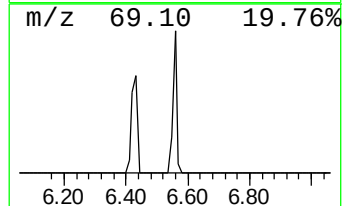
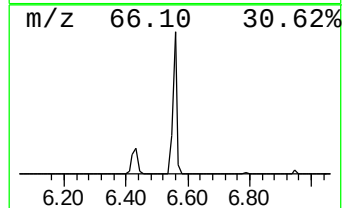
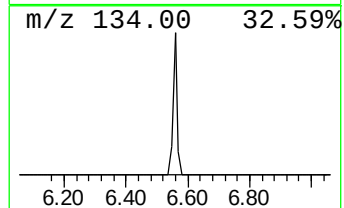
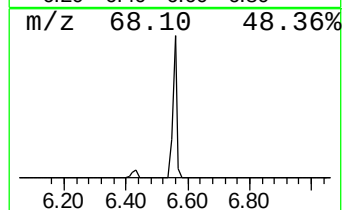
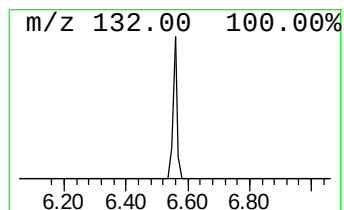
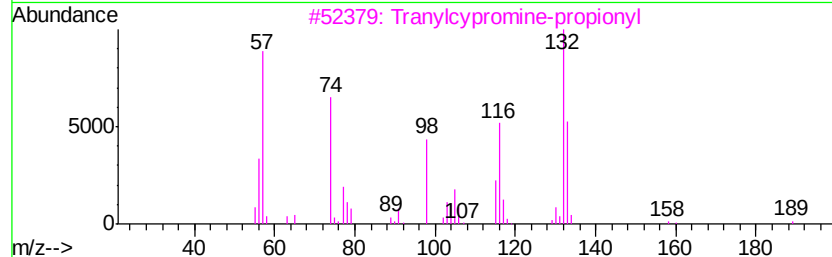
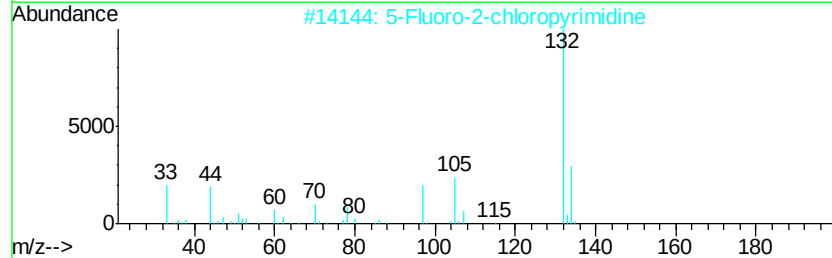
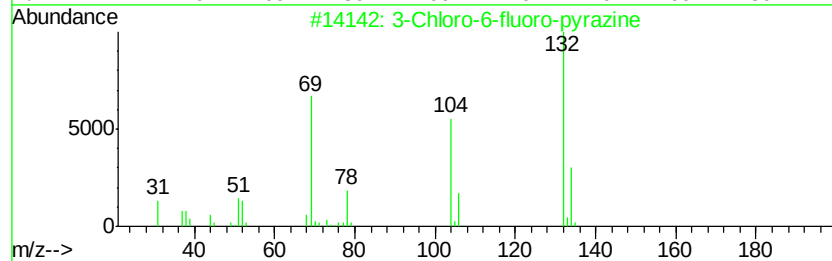
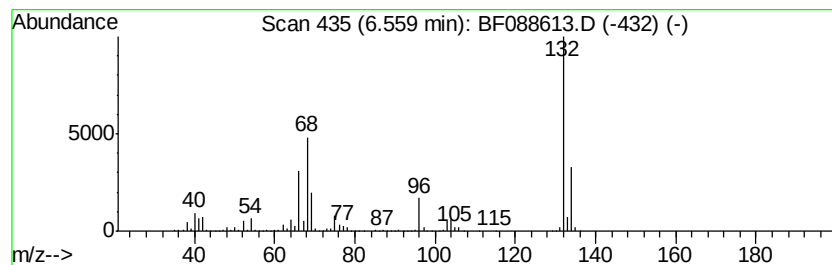
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	74.58 ng	2346580	1,4-Dichlorobenzene-d4	6.79

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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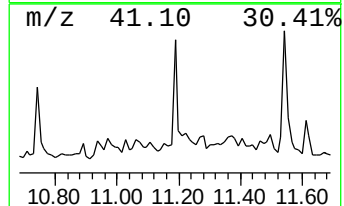
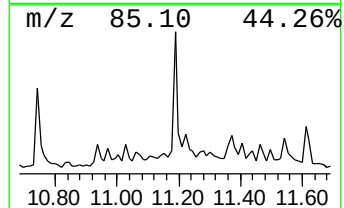
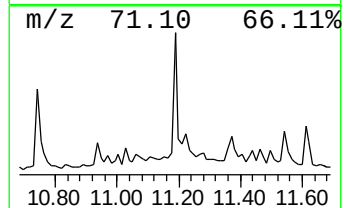
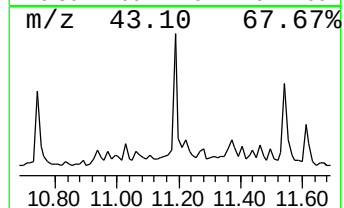
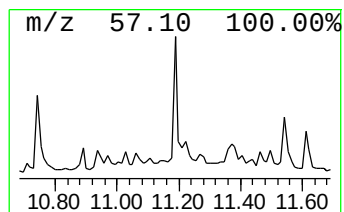
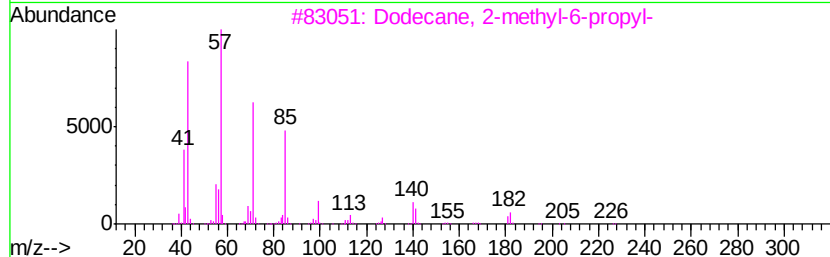
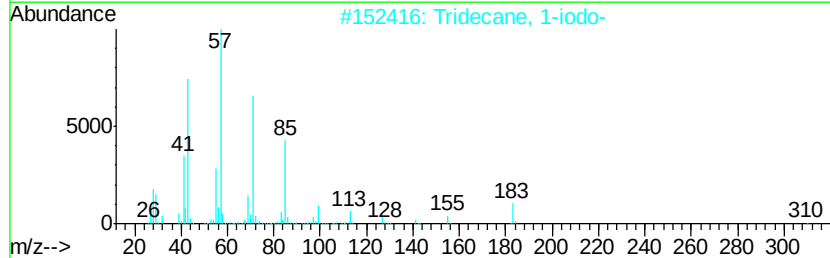
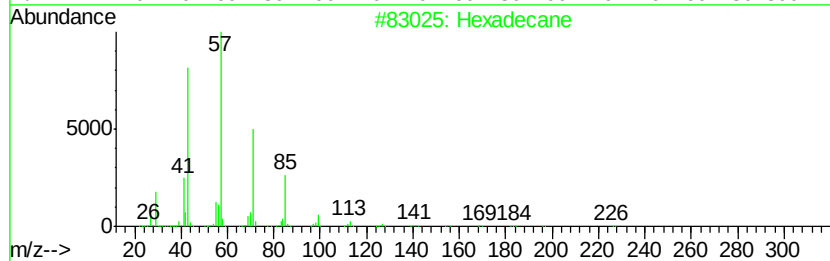
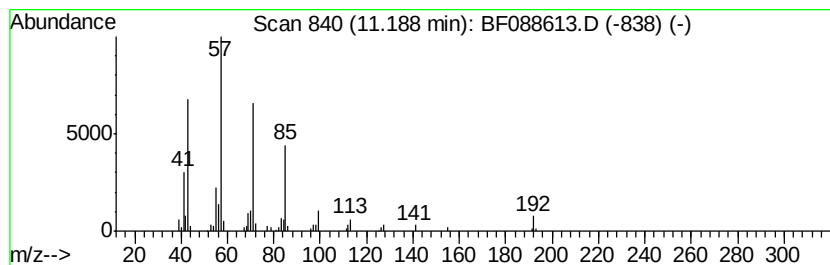
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.20 ng	87025	Phenanthrene-d10	11.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	90
2	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	86
3	Dodecane, 2-methyl-6-propyl-	226 C16H34	055045-08-4	72
4	Octacosane	394 C28H58	000630-02-4	72
5	Pentadecane	212 C15H32	000629-62-9	72



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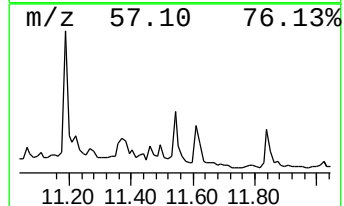
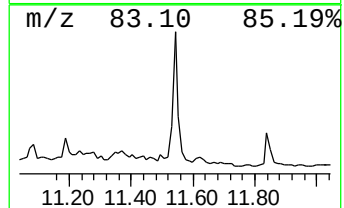
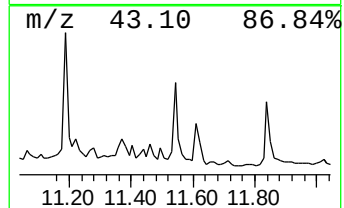
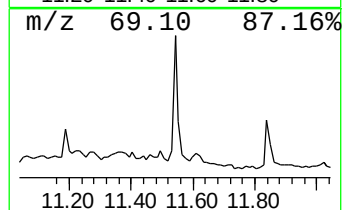
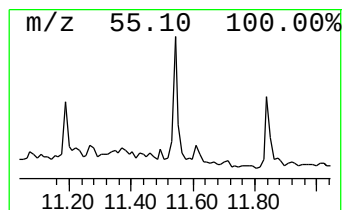
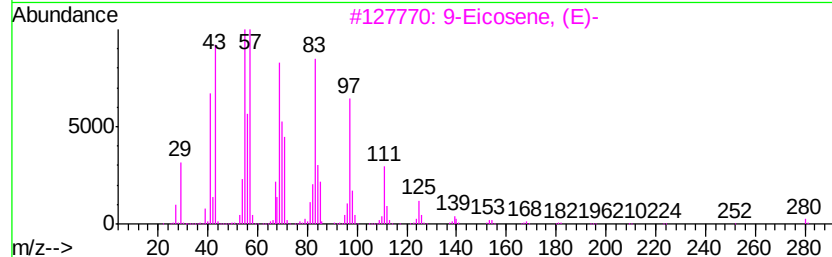
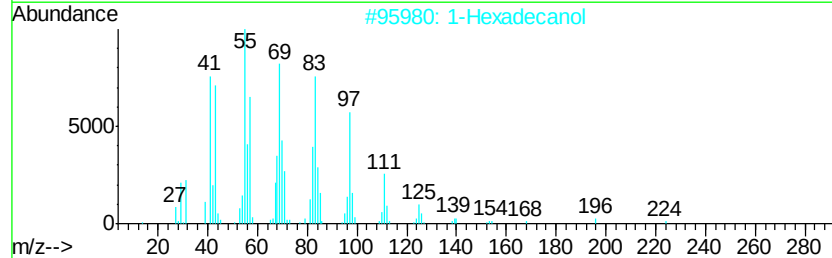
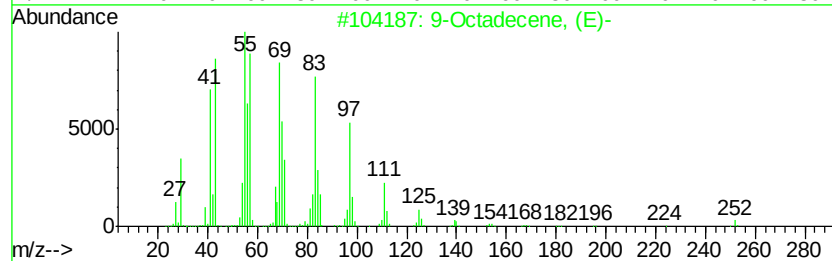
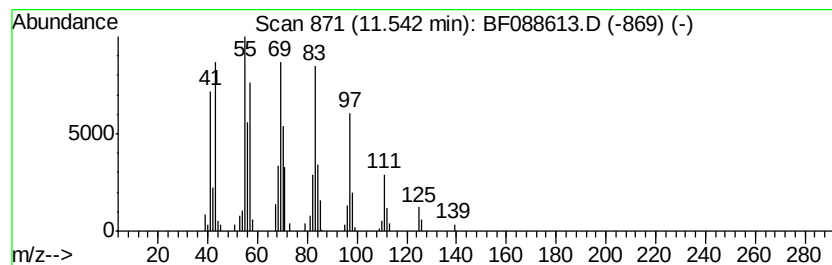
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.88 ng	113994	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5		11-Tricosene	322	C23H46	052078-56-5	90



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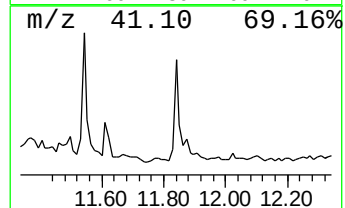
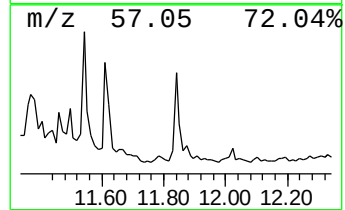
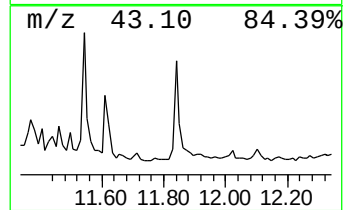
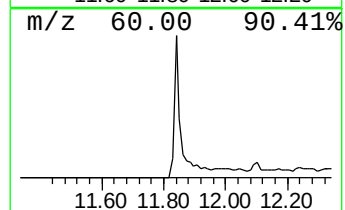
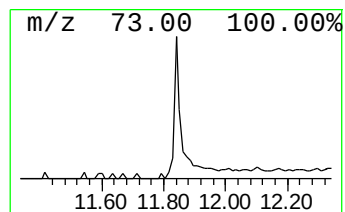
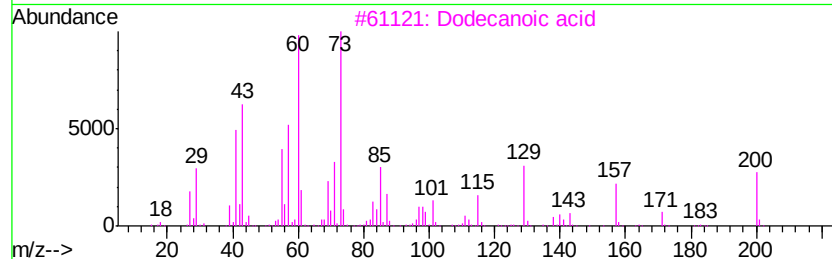
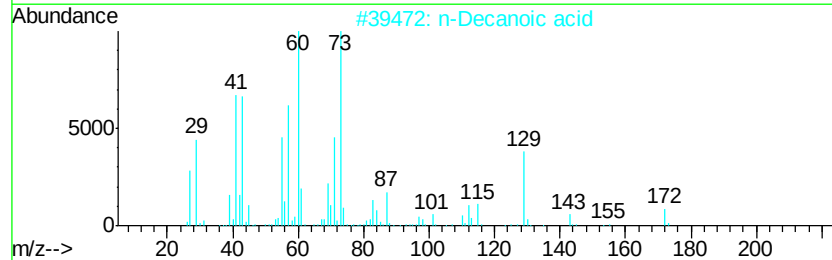
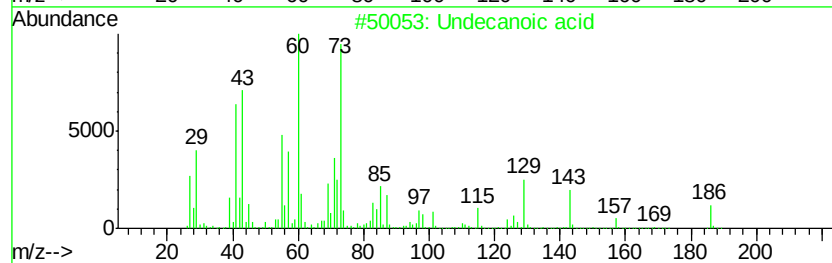
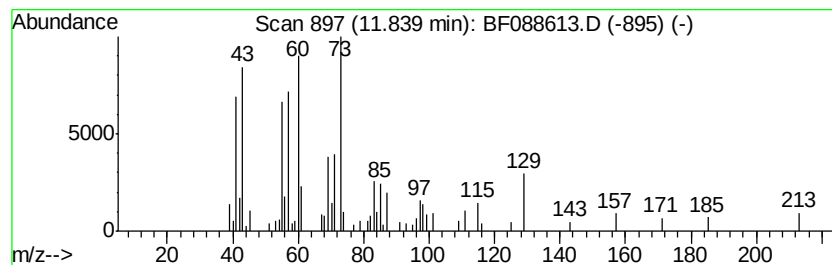
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Peak Number 8 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.84	2.58 ng	102128	Phenanthrene-d10	11.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86	
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59	
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53	
4	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	38	
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15	



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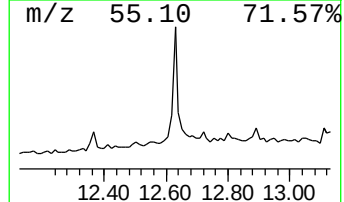
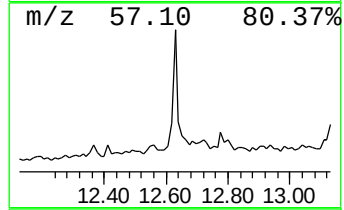
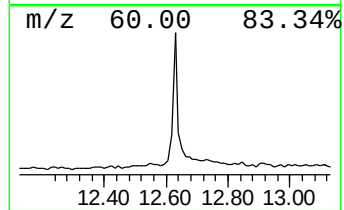
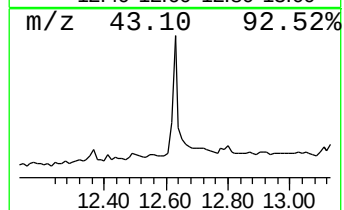
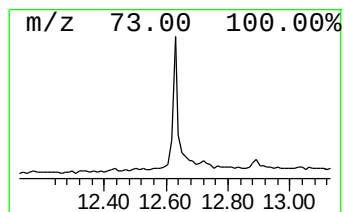
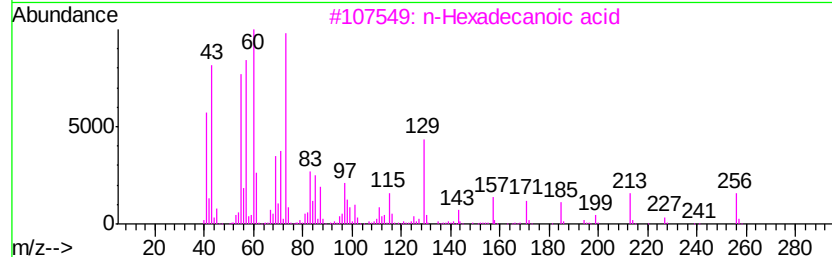
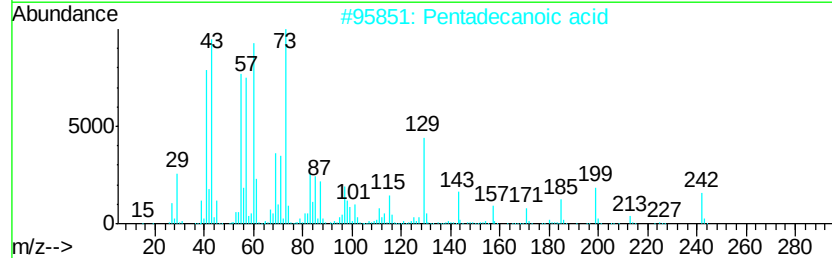
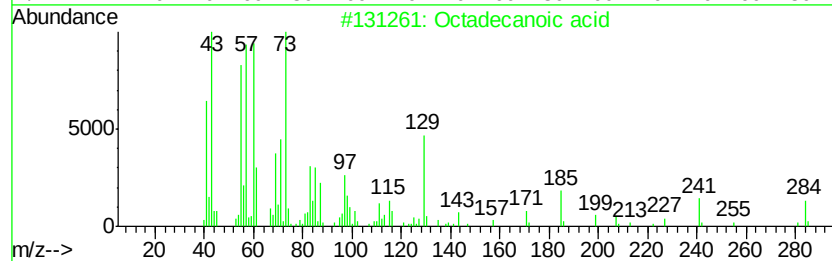
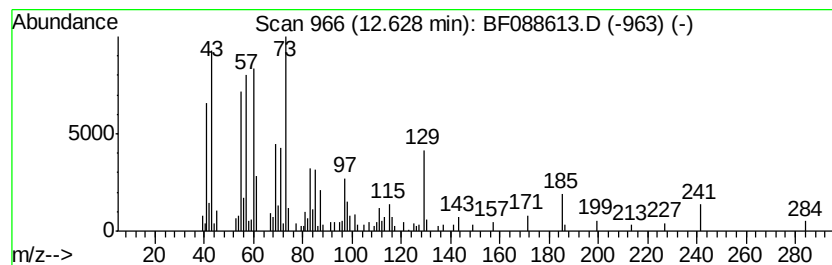
Instrument :
BNA_F
ClientSampleId :
K8-B2(0-11)C

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 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.63	4.49 ng	159809	Chrysene-d12		13.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088613.D
Acq On : 2 Jul 2016 13:16
Operator : UM/SJ
Sample : H3871-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K8-B2(0-11)C

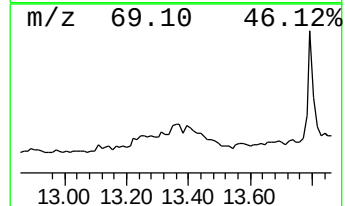
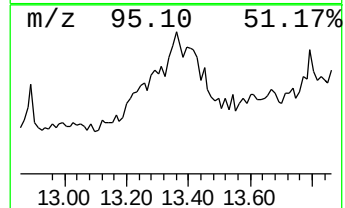
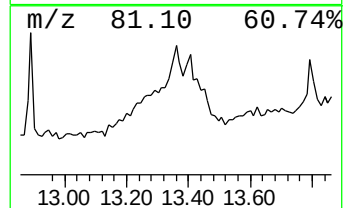
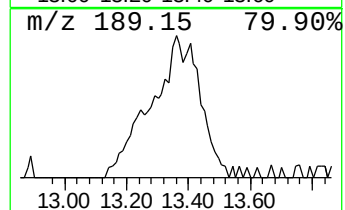
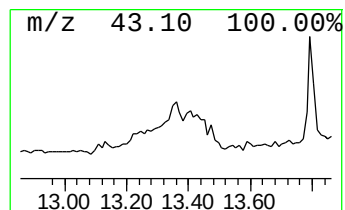
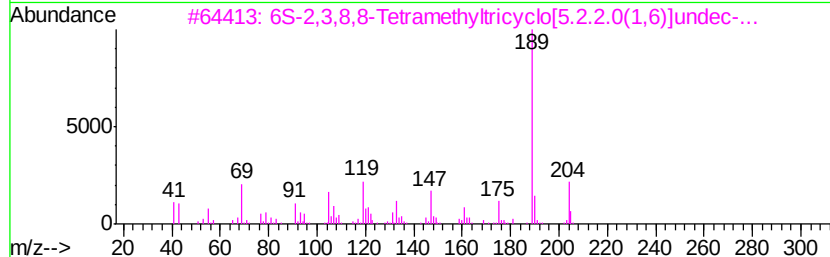
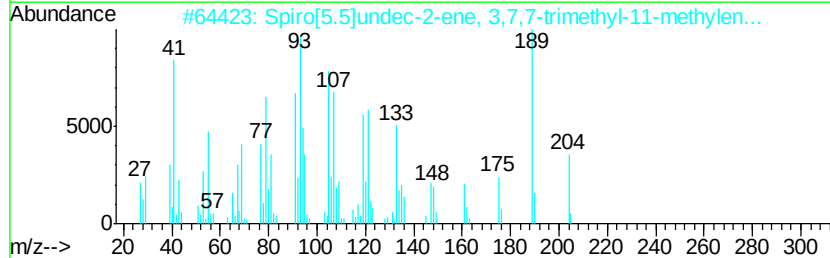
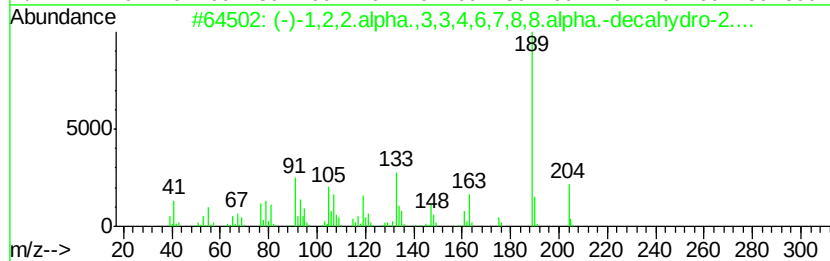
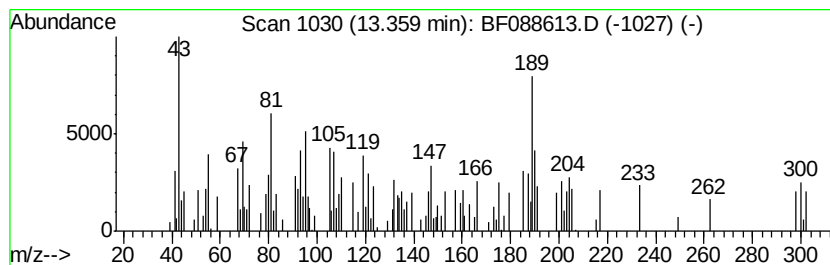
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.36 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.09 ng	74420	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(-)-1,2,2.alpha.,3,3,4,6,7,8,8.a...	204	C15H24	1000365-86-7	45
2		Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	35
3		6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	27
4		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	22
5		2,10,10-Trimethyltricyclo[7.1.1....	204	C14H200	1000210-81-9	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088613.D
Acq On : 2 Jul 2016 13:16
Operator : UM/SJ
Sample : H3871-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K8-B2(0-11)C

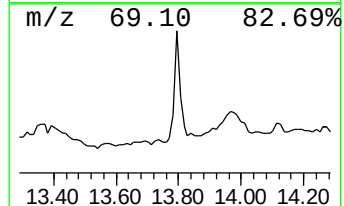
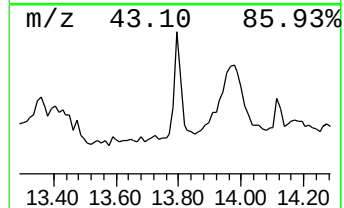
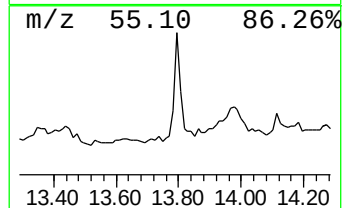
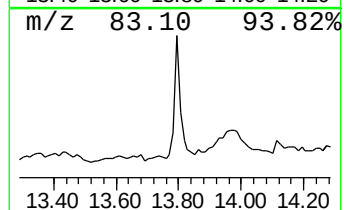
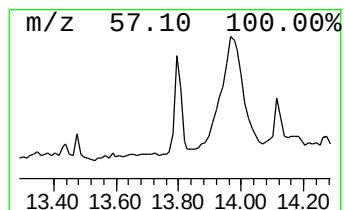
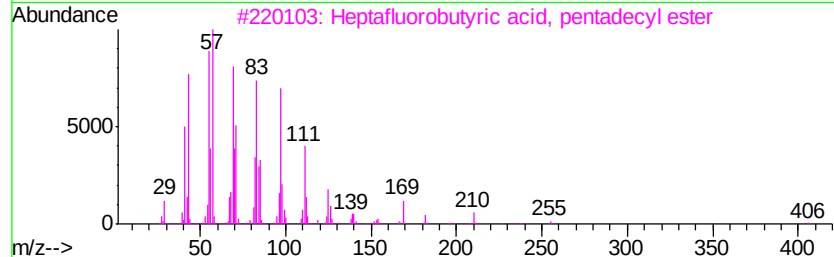
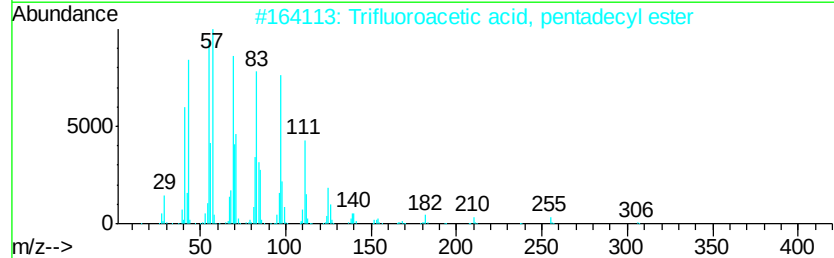
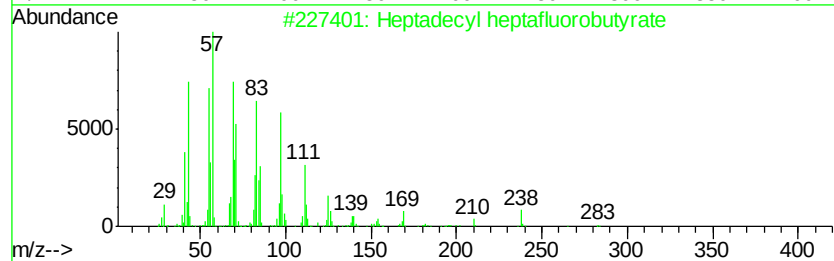
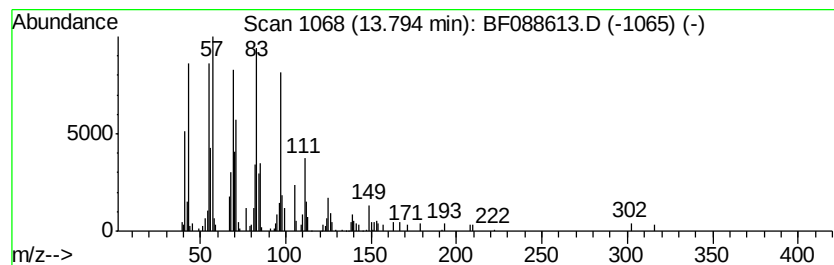
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.37 ng	262132	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
5		Trifluoroacetox hexadecane	338	C18H33F3O2	006222-03-3	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
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Sample : H3871-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K8-B2(0-11)C

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
unknown4.96	4.96	6.2	ng	194652	1	6.79	629300	20.0
unknown6.56	6.56	74.6	ng	2346580	1	6.79	629300	20.0
Hexadecane	11.19	2.2	ng	87025	4	11.30	792884	20.0
9-Octadecene, (E)-	11.54	2.9	ng	113994	4	11.30	792884	20.0
Undecanoic acid	11.84	2.6	ng	102128	4	11.30	792884	20.0
Octadecanoic acid	12.63	4.5	ng	159809	5	13.93	711328	20.0
unknown13.36	13.36	2.1	ng	74420	5	13.93	711328	20.0
Heptadecyl heptaf...	13.79	7.4	ng	262132	5	13.93	711328	20.0