

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
 Data File : BF087979.D
 Acq On : 13 Jun 2016 13:11
 Operator : UM/SJ
 Sample : H3438-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10-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-BF060716.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	322099	599782	20.93%	2.041%
2	1.861	22	24	37	rVB	1381104	2865410	100.00%	9.753%
3	3.073	128	130	142	rBV	21821	63800	2.23%	0.217%
4	4.970	293	296	302	rVB	107837	163216	5.70%	0.556%
5	5.393	330	333	335	rBV	1635595	2431247	84.85%	8.275%
6	6.433	420	424	426	rBV	2159052	2482648	86.64%	8.450%
7	6.559	432	435	437	rBV	2361243	2304160	80.41%	7.842%
8	6.787	453	455	458	rBV	799286	729005	25.44%	2.481%
9	6.947	466	469	471	rBV	2108235	1865558	65.11%	6.350%
10	7.359	502	505	507	rBV	1670095	1661302	57.98%	5.654%
11	7.462	510	514	520	rVB	27793	37476	1.31%	0.128%
12	8.079	565	568	570	rBV	1246161	1059521	36.98%	3.606%
13	9.165	660	663	665	rBV	2384213	2791601	97.42%	9.502%
14	9.553	695	697	699	rBV	836623	799436	27.90%	2.721%
15	9.839	719	722	724	rBV	879997	1155034	40.31%	3.931%
16	10.274	759	760	762	rVB	41616	29672	1.04%	0.101%
17	10.616	788	790	793	rBV2	1234026	1597077	55.74%	5.436%
18	10.742	799	801	806	rVB	46302	55373	1.93%	0.188%
19	11.188	838	840	842	rBV	49849	53505	1.87%	0.182%
20	11.314	849	851	853	rBV	1307150	1126577	39.32%	3.834%
21	11.622	875	878	880	rBV	238341	240099	8.38%	0.817%
22	11.851	896	898	900	rBV	69612	68139	2.38%	0.232%
23	12.022	911	913	918	rVB	48273	42531	1.48%	0.145%
24	12.411	945	947	949	rVB	63036	54843	1.91%	0.187%
25	12.514	955	956	958	rBV	37967	51762	1.81%	0.176%
26	12.731	973	975	978	rBV2	310199	295212	10.30%	1.005%
27	12.811	978	982	983	rBV3	22496	35207	1.23%	0.120%
28	12.902	987	990	992	rBV	2195645	2108153	73.57%	7.175%
29	13.440	1034	1037	1038	rBV	133957	154554	5.39%	0.526%
30	13.817	1067	1070	1078	rBV	66673	180770	6.31%	0.615%
31	13.942	1078	1081	1085	rVV	1031403	1014718	35.41%	3.454%
32	14.457	1121	1126	1134	rBV2	58878	201170	7.02%	0.685%
33	14.708	1143	1148	1151	rBV2	23498	71998	2.51%	0.245%
34	14.948	1168	1169	1175	rVB	23625	42293	1.48%	0.144%

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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	15.097	1179	1182	1192	rVB3	31114	122772	4.28%	0.418%
36	15.360	1202	1205	1207	rBV	577044	794553	27.73%	2.704%
37	18.206	1449	1454	1460	rVB8	7077	30387	1.06%	0.103%

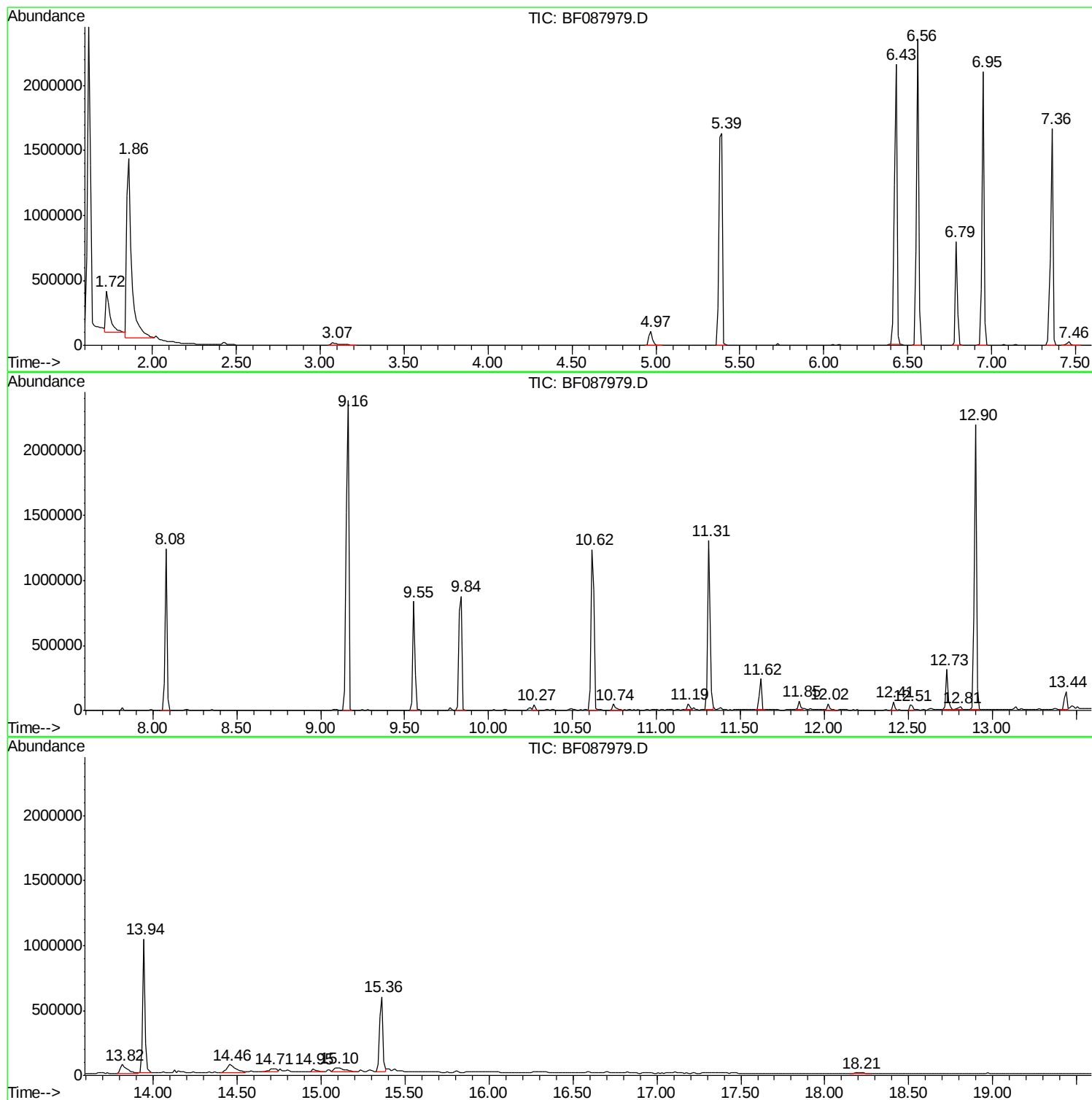
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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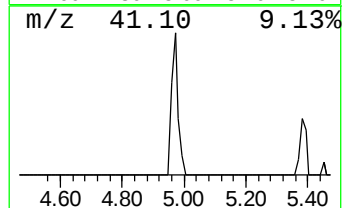
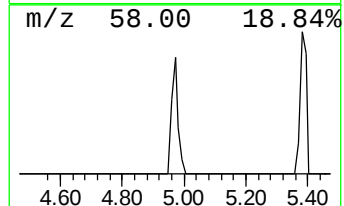
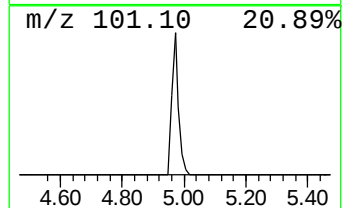
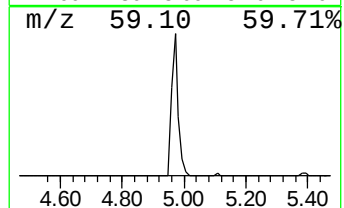
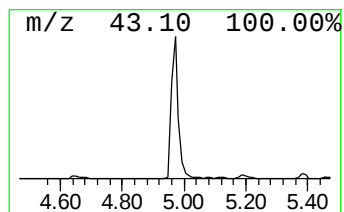
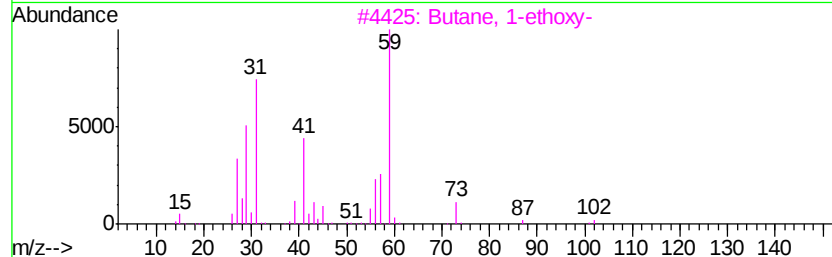
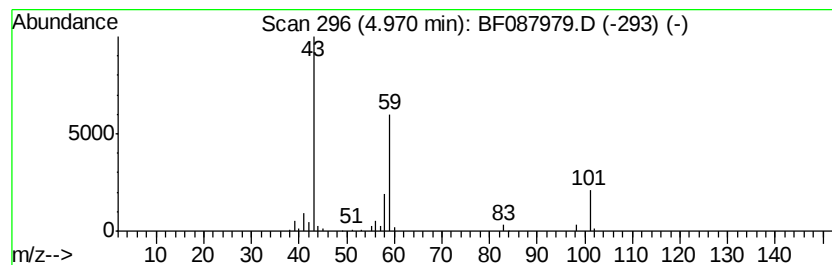
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	4.48 ng	163216	1,4-Dichlorobenzene-d4	6.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	Acetone	58	C3H6O	000067-64-1	9	



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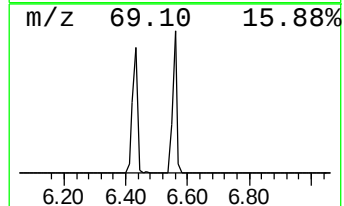
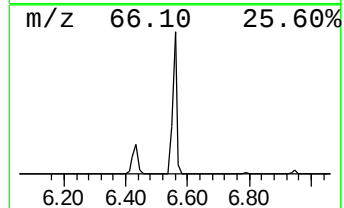
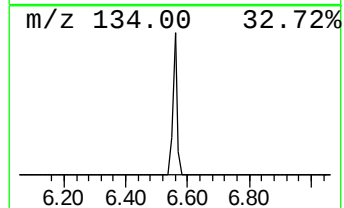
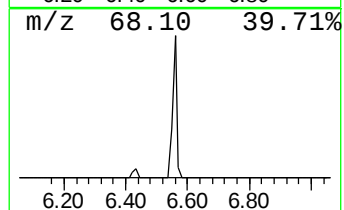
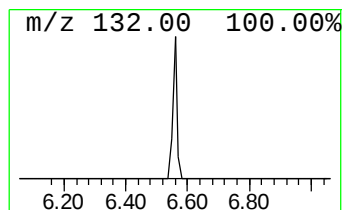
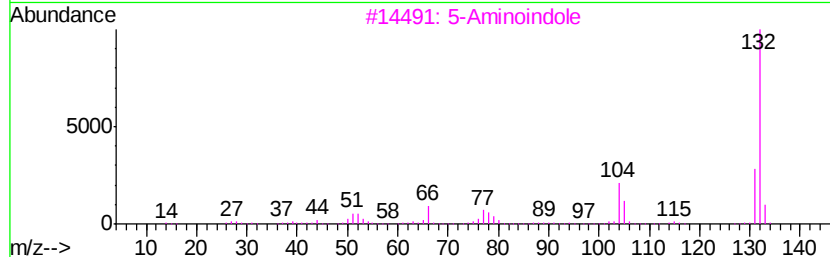
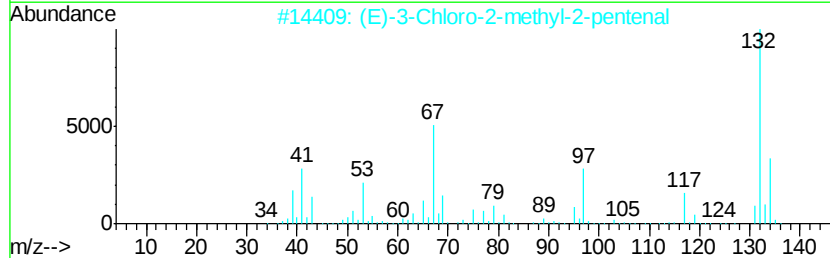
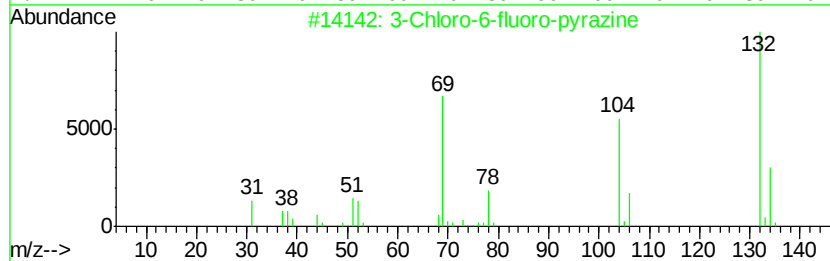
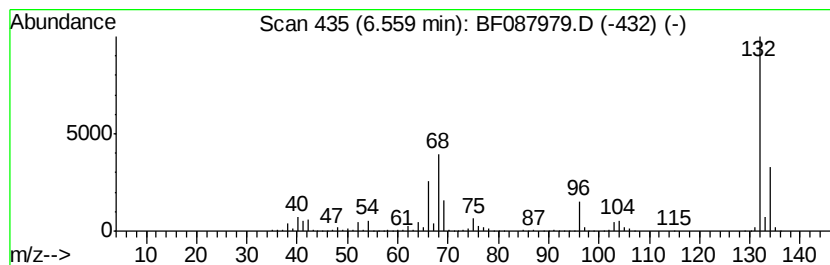
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	63.21 ng	2304160	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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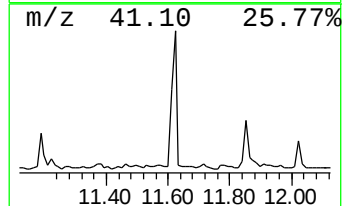
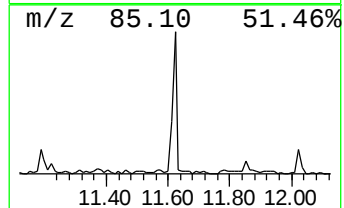
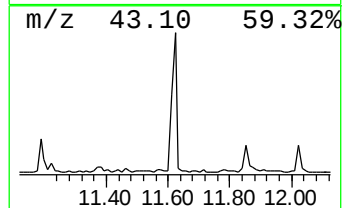
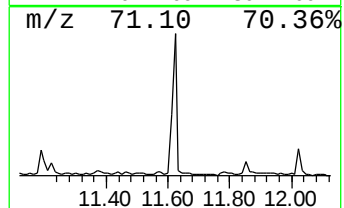
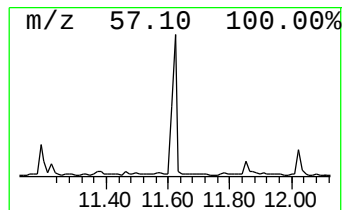
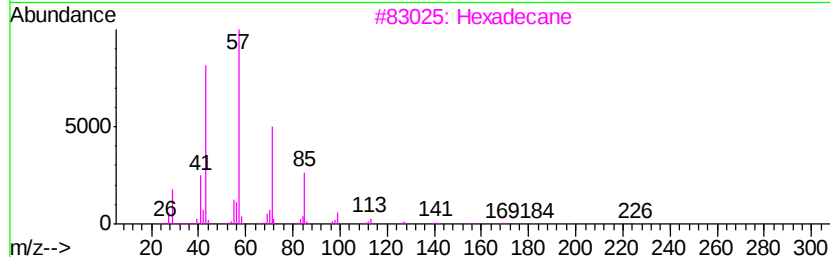
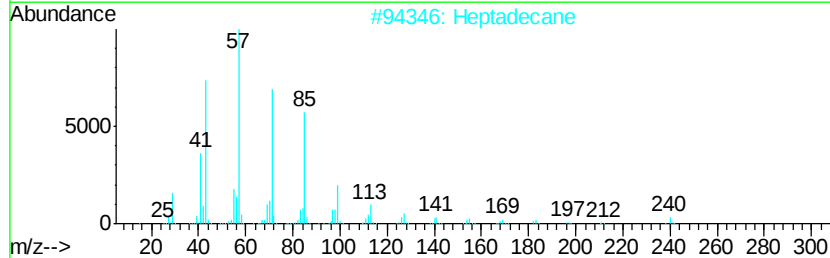
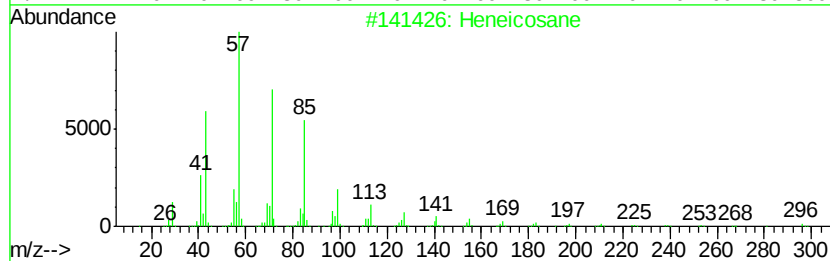
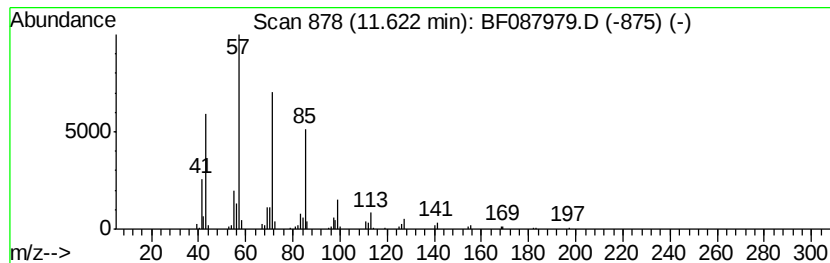
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	4.26 ng	240099	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Hexadecane	226	C16H34	000544-76-3	86
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



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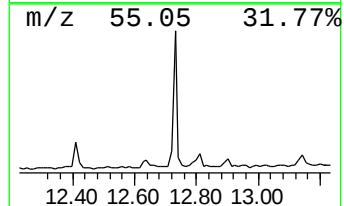
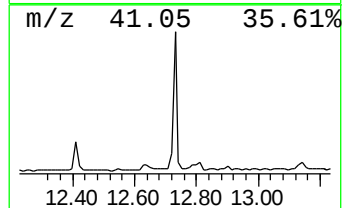
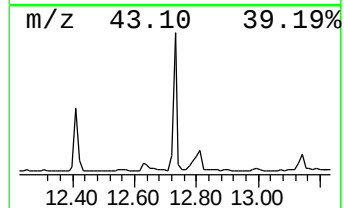
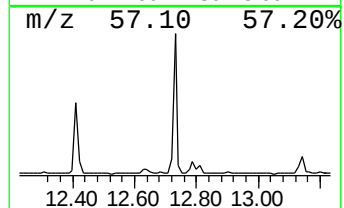
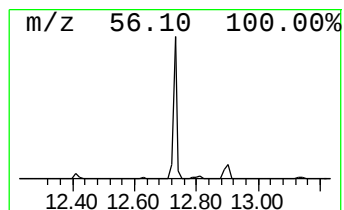
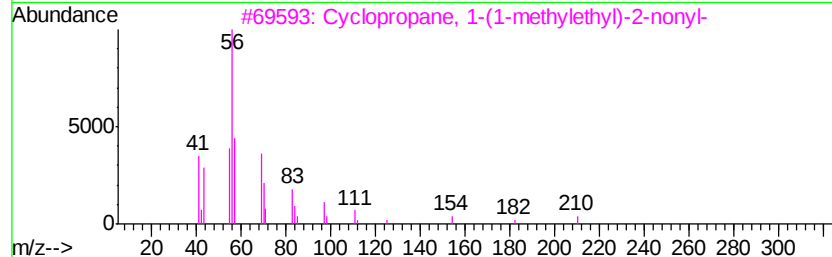
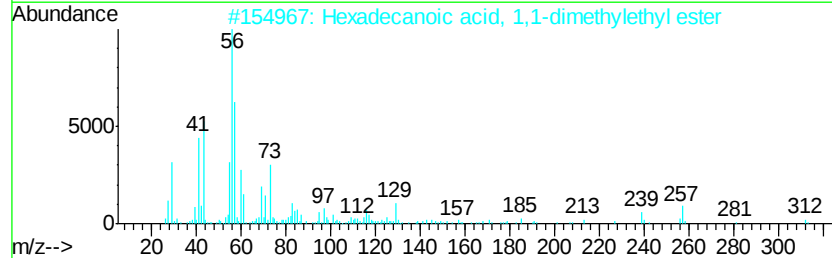
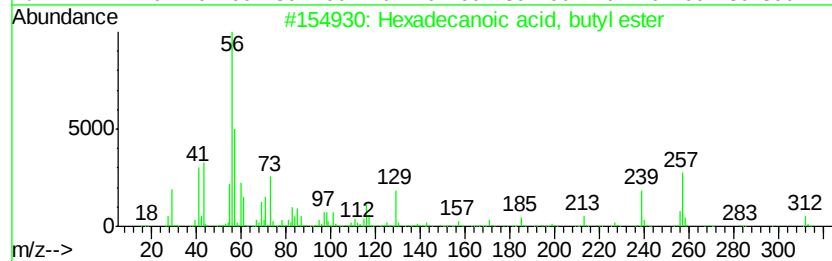
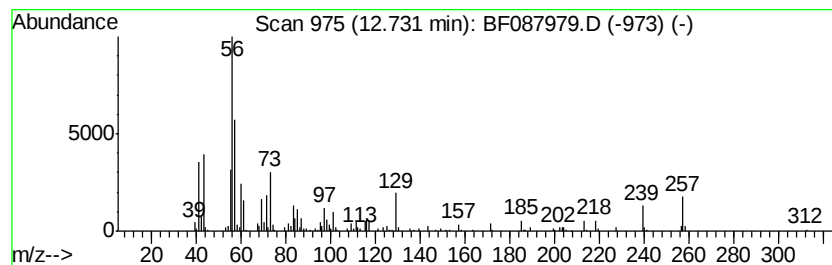
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.73	5.82 ng	295212	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Cvclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	35



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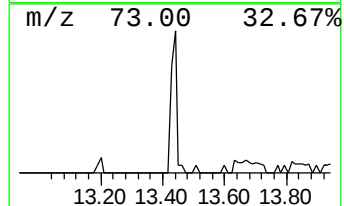
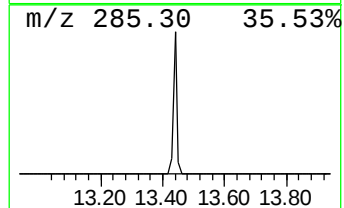
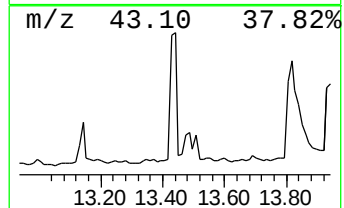
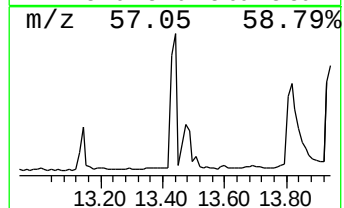
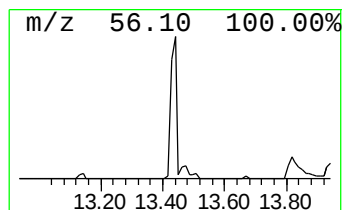
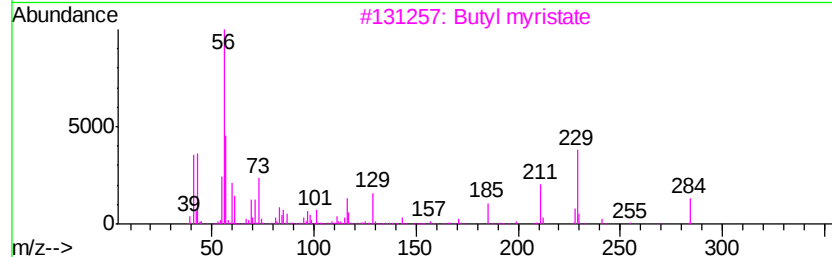
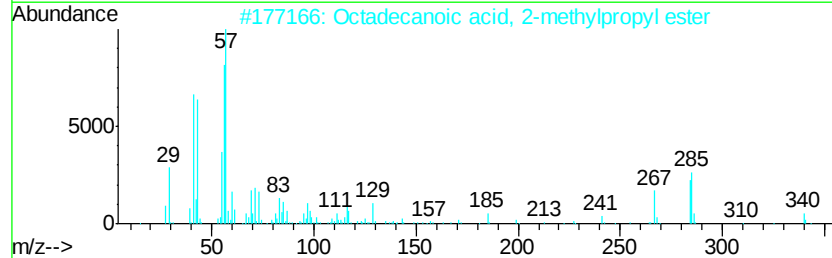
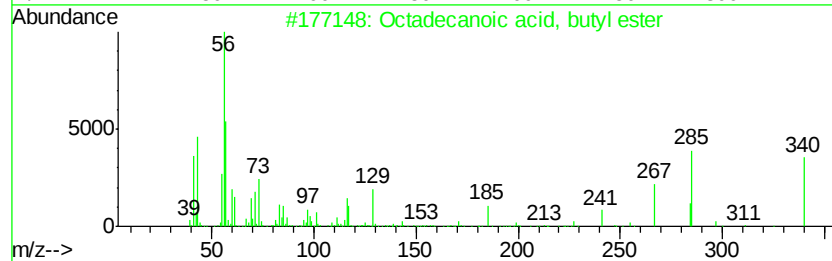
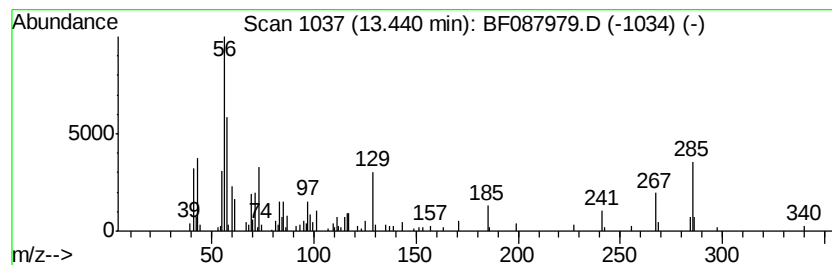
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Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	3.05 ng	154554	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	83
3		Butyl myristate	284	C18H36O2	000110-36-1	47
4		Nipecotic acid	129	C6H11NO2	000498-95-3	43
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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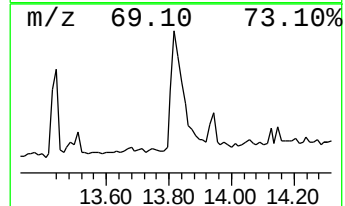
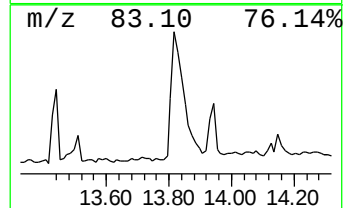
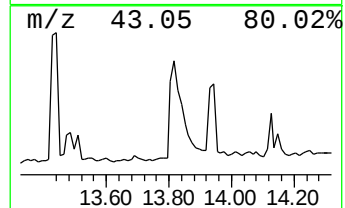
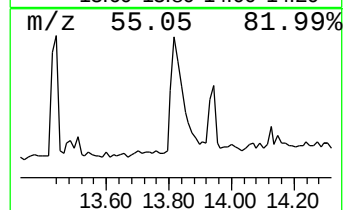
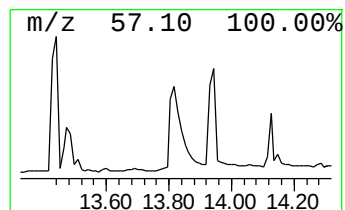
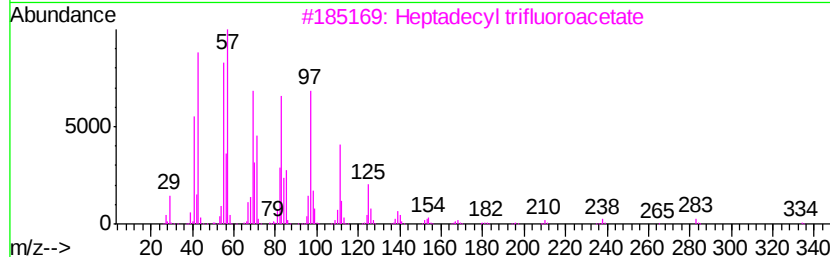
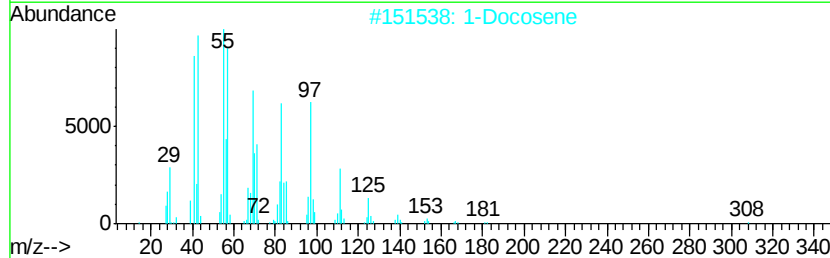
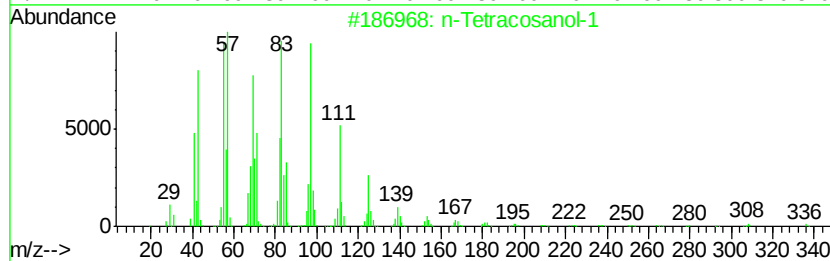
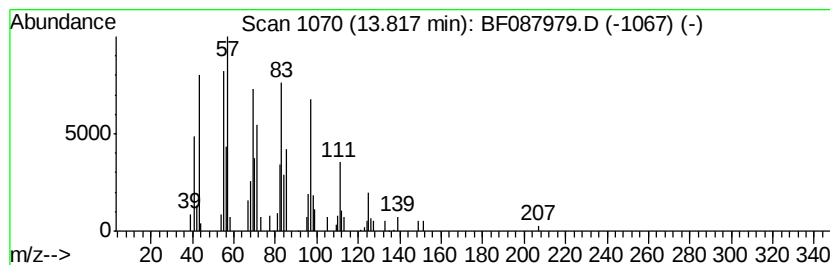
Instrument :
BNA_F
ClientSampleId :
SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.56 ng	180770	Chrysene-d12	13.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Tetracosanol-1	354 C24H50O	000506-51-4	93
2	1-Docosene	308 C22H44	001599-67-3	90
3	Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0	90
4	Nonadecyl pentafluoropropionate	430 C22H39F5O2	1000351-88-8	90
5	Heneicosyl heptafluorobutyrate	508 C25H43F7O2	1000351-83-8	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087979.D
Acq On : 13 Jun 2016 13:11
Operator : UM/SJ
Sample : H3438-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP

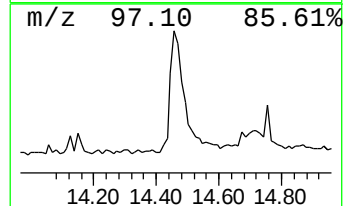
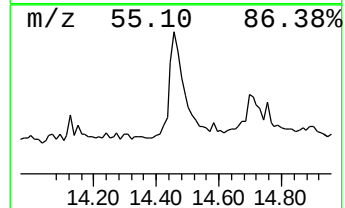
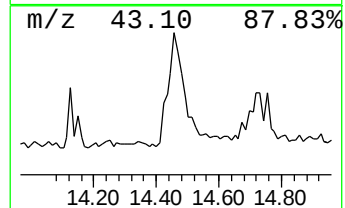
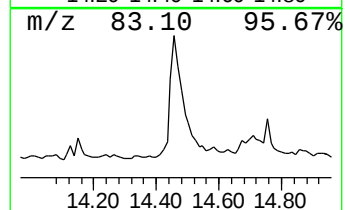
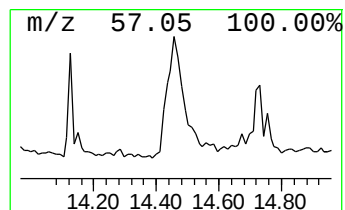
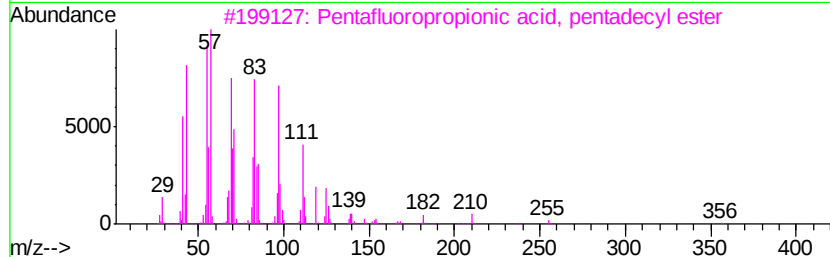
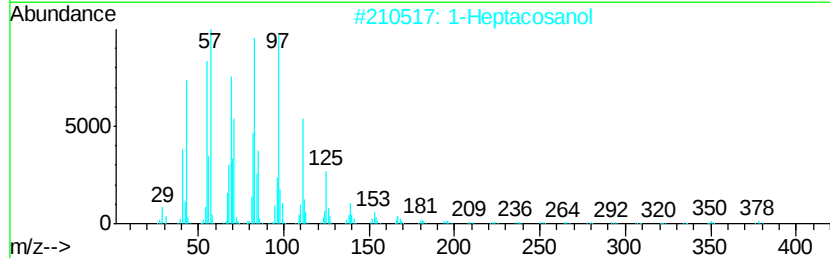
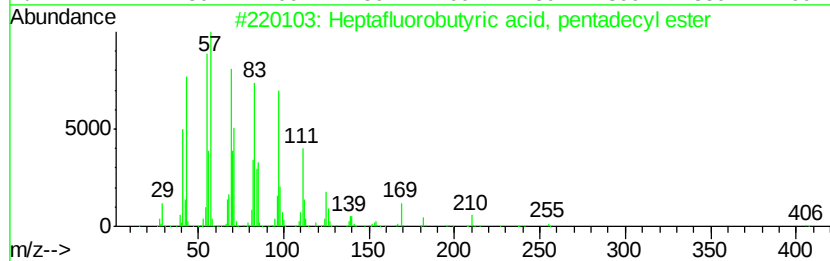
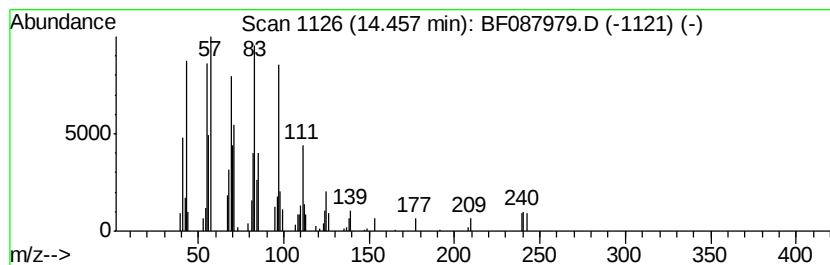
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptafluorobutyric acid, pe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.97 ng	201170	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	95
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
Data File : BF087979.D
Acq On : 13 Jun 2016 13:11
Operator : UM/SJ
Sample : H3438-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

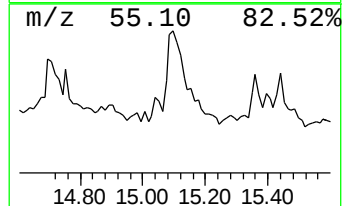
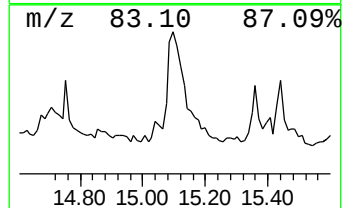
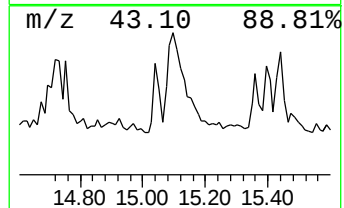
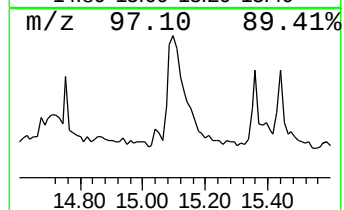
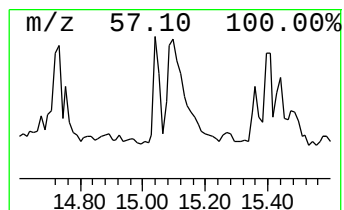
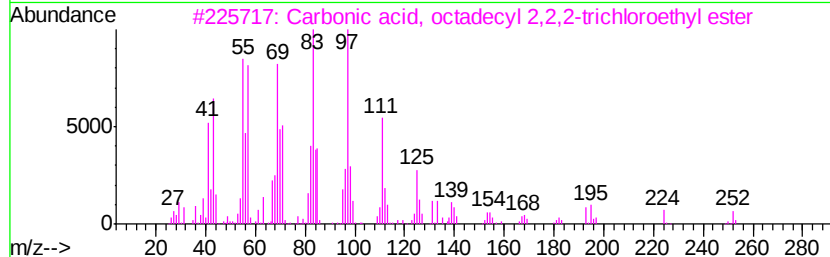
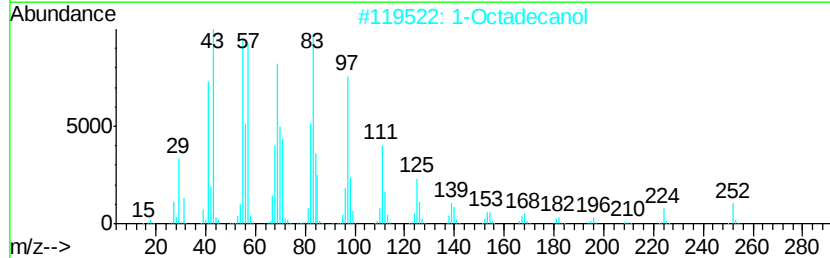
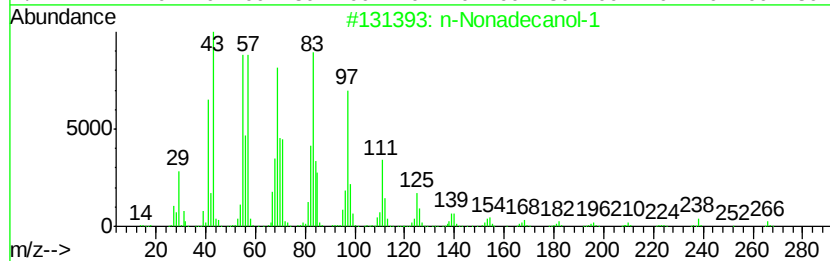
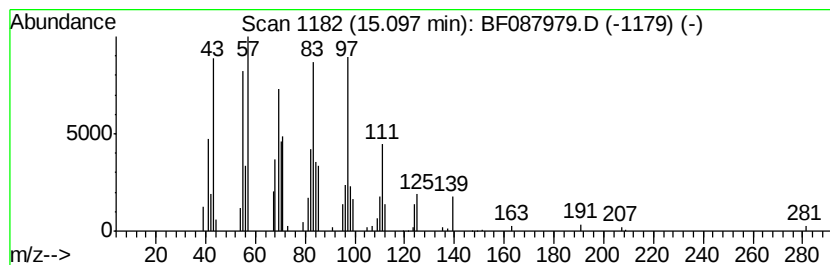
Instrument :
BNA_F
ClientSampleId :
SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.09 ng	122772	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Nonadecanol-1	284 C19H40O	001454-84-8	94
2	1-Octadecanol	270 C18H38O	000112-92-5	91
3	Carbonic acid, octadecyl 2,2,2-t...	444 C21H39Cl3O3	1000314-56-3	91
4	Pentafluoropropionic acid, octad...	416 C21H37F5O2	959261-25-7	91
5	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061316\
Data File : BF087979.D
Acq On : 13 Jun 2016 13:11
Operator : UM/SJ
Sample : H3438-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.97	4.5 ng		163216	1	6.79	729005	20.0
unknown6.56	6.56	63.2 ng		2304160	1	6.79	729005	20.0
Heneicosane	11.62	4.3 ng		240099	4	11.31	1126580	20.0
Hexadecanoic acid...	12.73	5.8 ng		295212	5	13.94	1014720	20.0
Octadecanoic acid...	13.44	3.0 ng		154554	5	13.94	1014720	20.0
n-Tetracosanol-1	13.82	3.6 ng		180770	5	13.94	1014720	20.0
Heptafluorobutyri...	14.46	4.0 ng		201170	5	13.94	1014720	20.0
n-Nonadecanol-1	15.10	3.1 ng		122772	6	15.36	794553	20.0