

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
 Data File : BF098607.D
 Acq On : 18 Sep 2017 17:36
 Operator : SJ/JU
 Sample : I5244-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-TP-106-X(0-5)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-BF091117.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	4.822	461	465	482	rBV	207173	351278	10.35%	1.207%
2	5.246	533	537	553	rBV	3155382	3335703	98.28%	11.457%
3	5.446	568	571	578	rBV	53698	64378	1.90%	0.221%
4	6.293	710	715	718	rBV	3108213	3225172	95.02%	11.077%
5	6.410	730	735	738	rBV	3870378	3394098	100.00%	11.658%
6	6.469	741	745	749	rVB	47061	47003	1.38%	0.161%
7	6.634	769	773	779	rVB	843086	687890	20.27%	2.363%
8	6.787	795	799	803	rBV	2359651	2278170	67.12%	7.825%
9	7.204	865	870	873	rBV	1993006	2079335	61.26%	7.142%
10	7.916	987	991	1001	rBV	1128019	940050	27.70%	3.229%
11	8.992	1169	1174	1177	rBV	3177931	2950695	86.94%	10.135%
12	9.392	1238	1242	1245	rBV	482058	362371	10.68%	1.245%
13	9.669	1281	1289	1293	rBV	1057270	995788	29.34%	3.420%
14	10.457	1419	1423	1432	rBV	2062149	1929762	56.86%	6.628%
15	11.151	1537	1541	1543	rBV	900648	847610	24.97%	2.911%
16	11.169	1543	1544	1548	rVB	91147	64514	1.90%	0.222%
17	11.757	1641	1644	1647	rBV	37559	40232	1.19%	0.138%
18	12.357	1742	1746	1750	rBV	255091	222619	6.56%	0.765%
19	12.586	1775	1785	1788	rBV	237339	273227	8.05%	0.938%
20	12.733	1805	1810	1813	rBV	2510456	2139814	63.05%	7.350%
21	12.804	1819	1822	1827	rVB4	27446	42395	1.25%	0.146%
22	13.016	1855	1858	1865	rVB2	32701	40160	1.18%	0.138%
23	13.351	1913	1915	1921	rVB2	37224	39131	1.15%	0.134%
24	13.627	1959	1962	1970	rVB2	132223	169883	5.01%	0.583%
25	13.780	1980	1988	1991	rBV2	736824	826958	24.36%	2.840%
26	13.810	1991	1993	1996	rVB	108403	93851	2.77%	0.322%
27	14.251	2063	2068	2073	rBV9	34609	70989	2.09%	0.244%
28	14.527	2112	2115	2121	rBV3	104321	137834	4.06%	0.473%
29	14.786	2156	2159	2163	rBV	120723	187114	5.51%	0.643%
30	14.851	2167	2170	2174	rVB2	41470	47832	1.41%	0.164%
31	15.063	2203	2206	2213	rVB	82588	94980	2.80%	0.326%
32	15.121	2213	2216	2221	rBV	107947	121027	3.57%	0.416%
33	15.180	2221	2226	2233	rBV	470883	616229	18.16%	2.117%
34	15.574	2290	2293	2297	rVB3	59927	77482	2.28%	0.266%

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SASP2P-TP-106-X(0-5)COMP

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	16.021	2365	2369	2377	rVB2	58187	93777	2.76%	0.322%
36	16.504	2448	2451	2454	rBV2	39247	57619	1.70%	0.198%
37	16.904	2515	2519	2526	rVB3	38396	76680	2.26%	0.263%
38	17.139	2557	2559	2568	rVB4	41761	90991	2.68%	0.313%

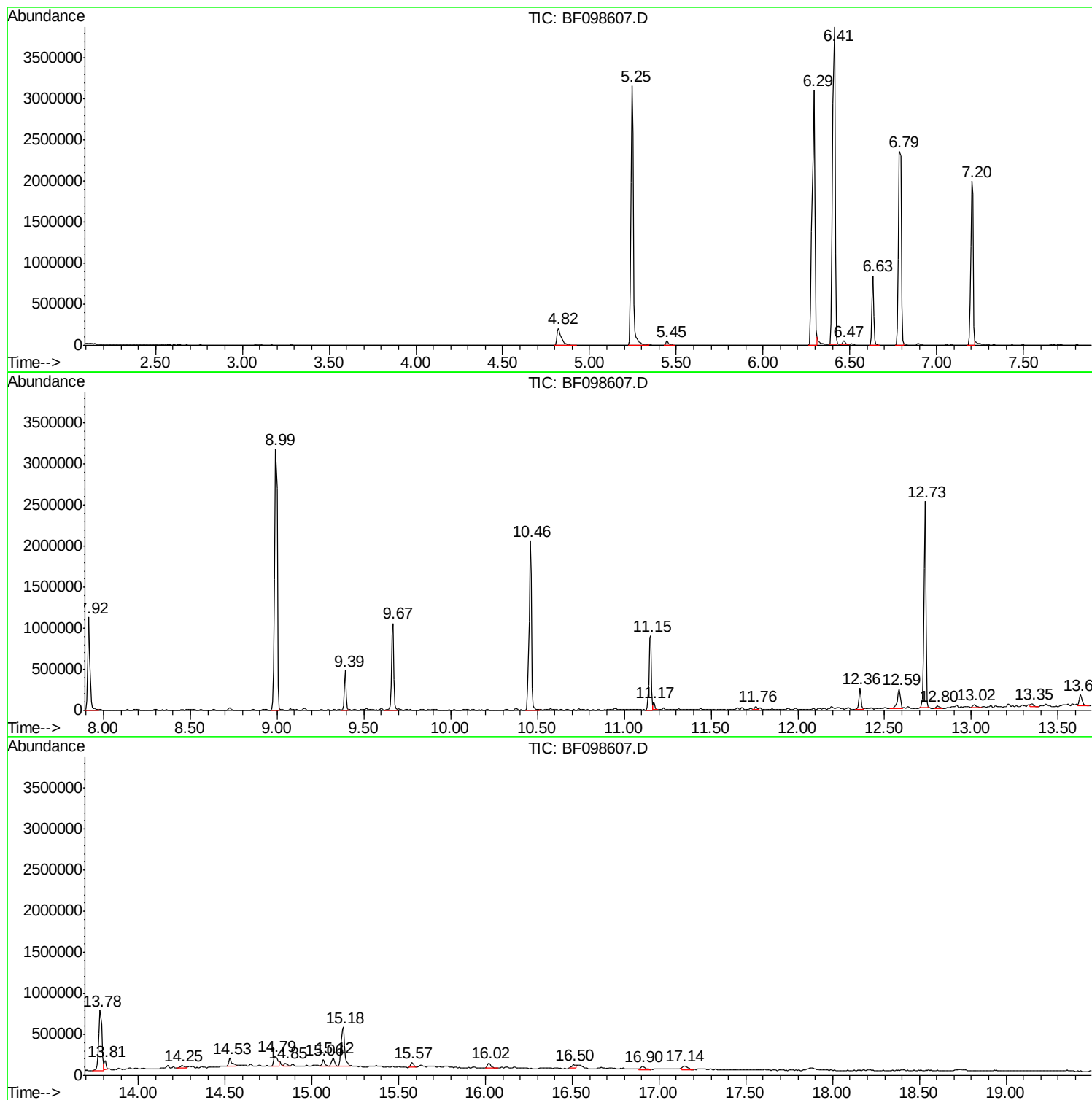
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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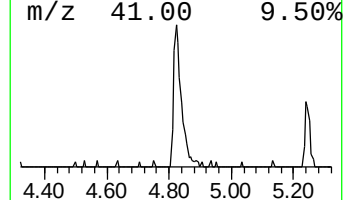
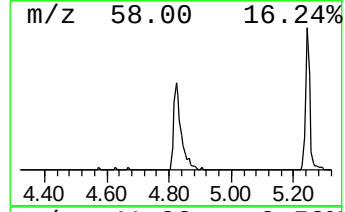
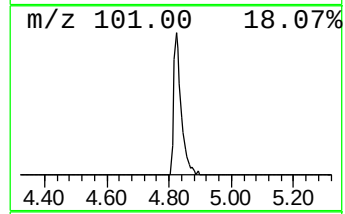
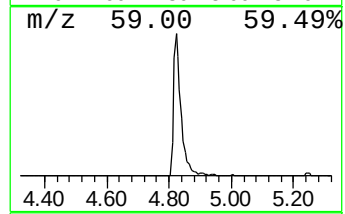
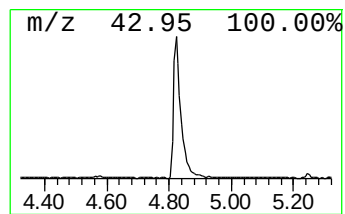
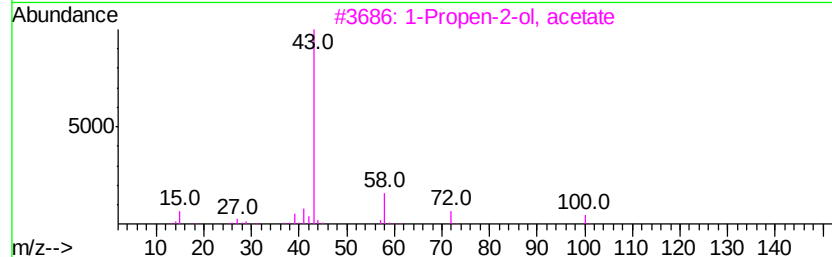
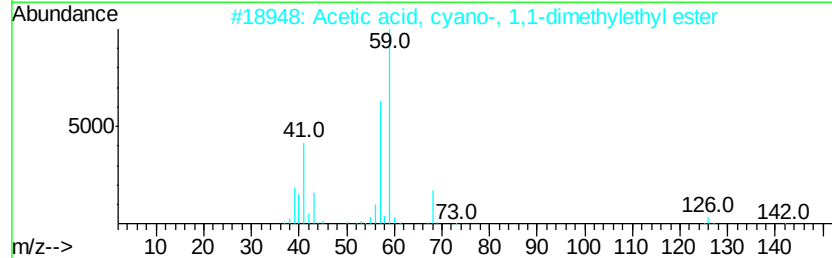
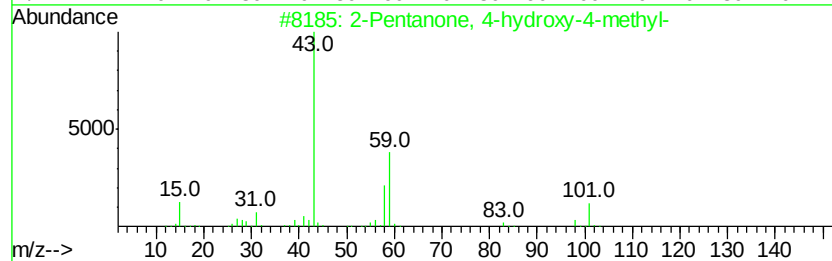
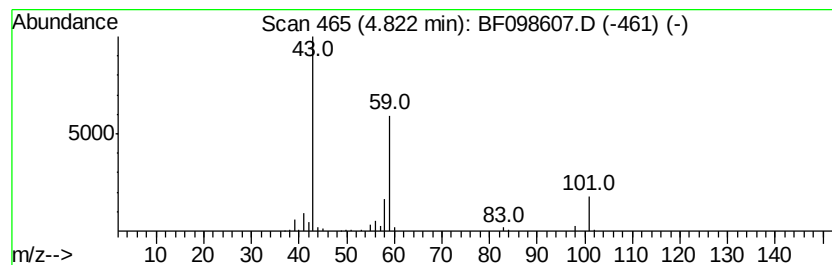
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	10.21 ng	351278	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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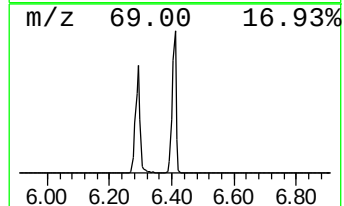
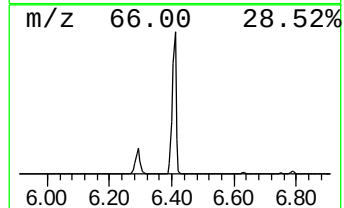
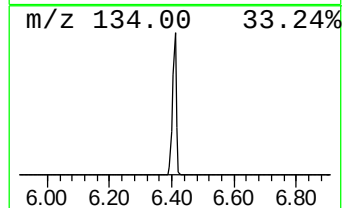
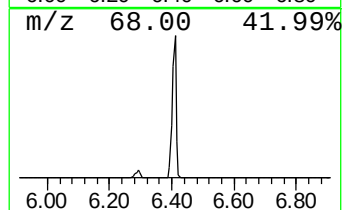
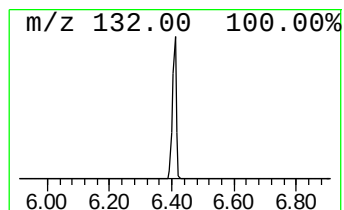
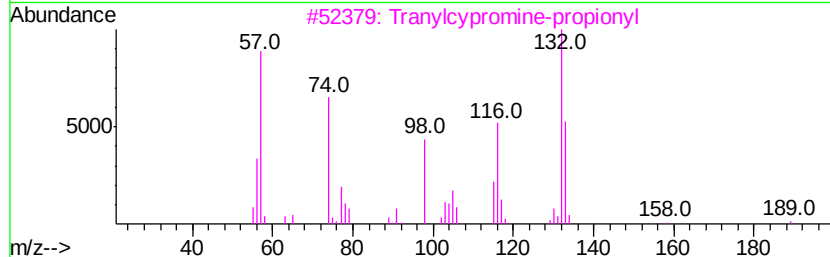
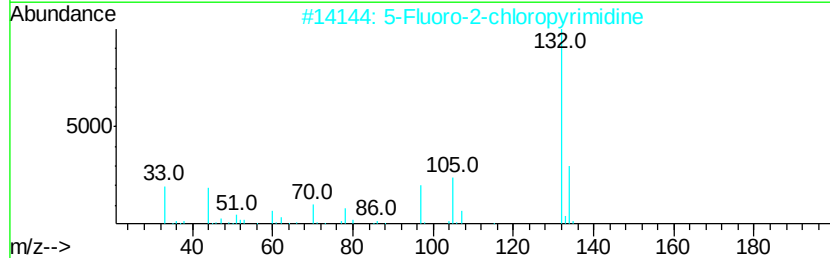
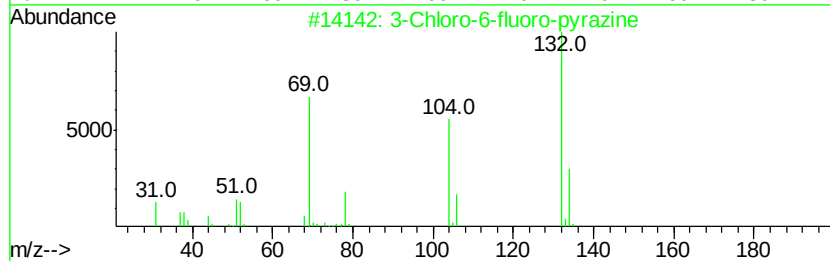
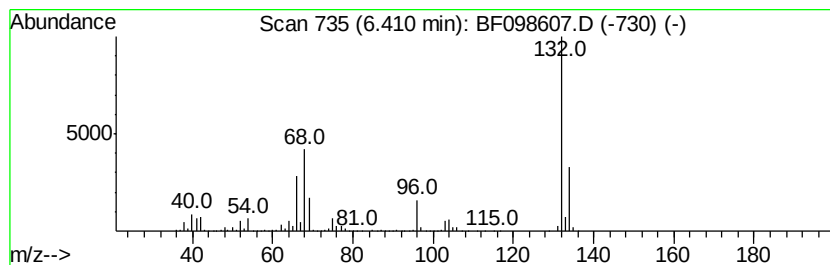
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	98.68 ng	3394100	1,4-Dichlorobenzene-d4	6.63

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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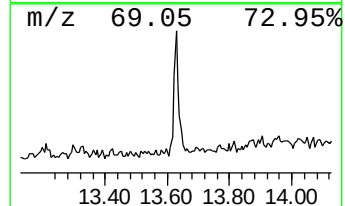
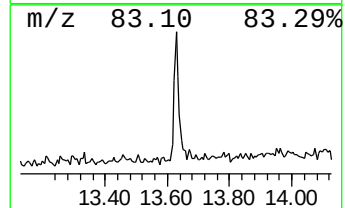
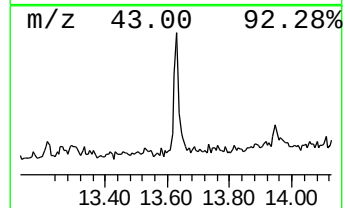
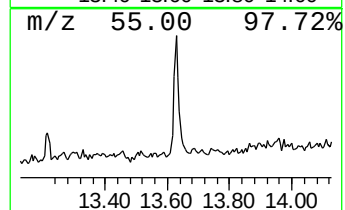
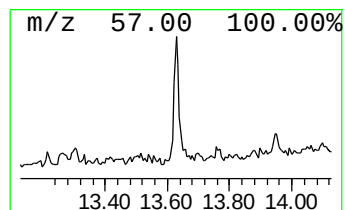
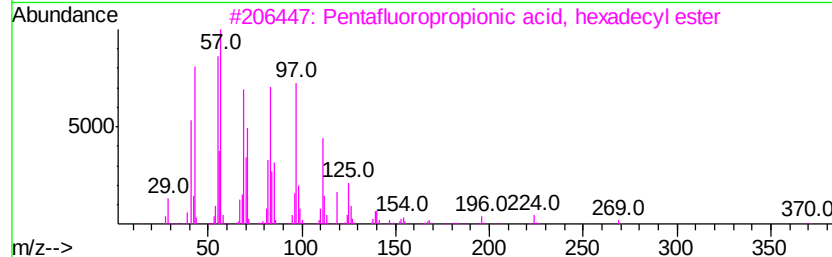
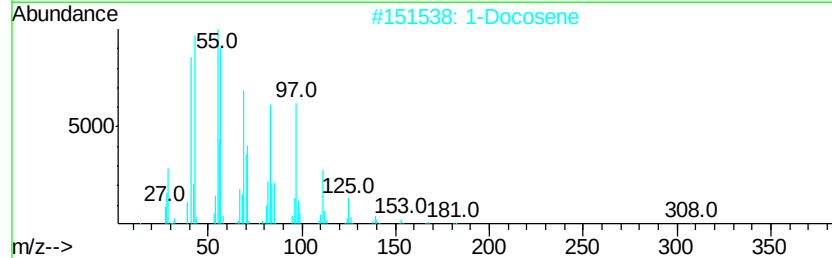
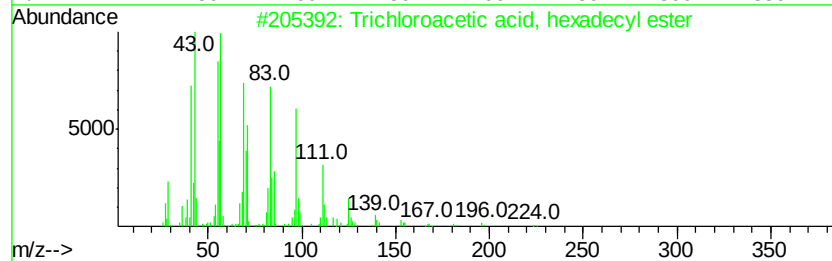
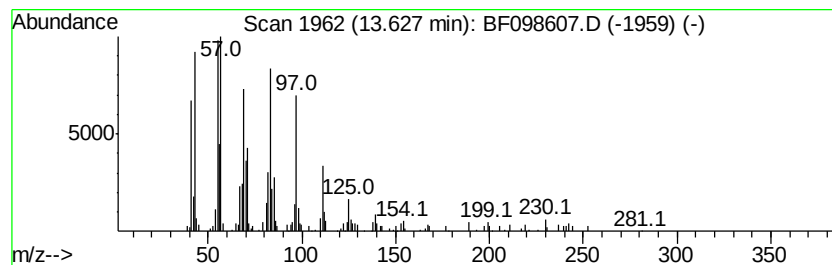
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.63	4.11 ng	169883	Chrysene-d12	13.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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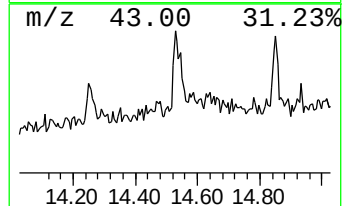
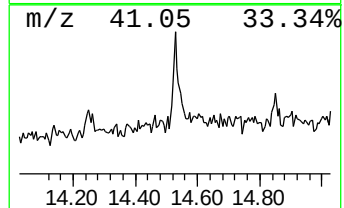
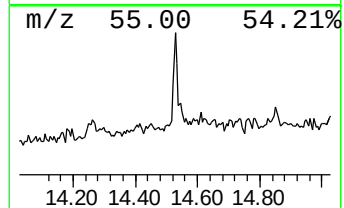
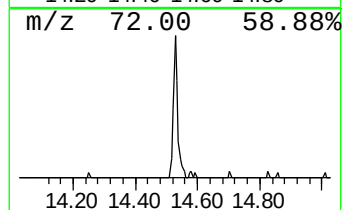
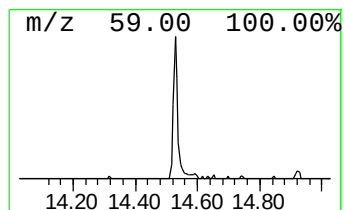
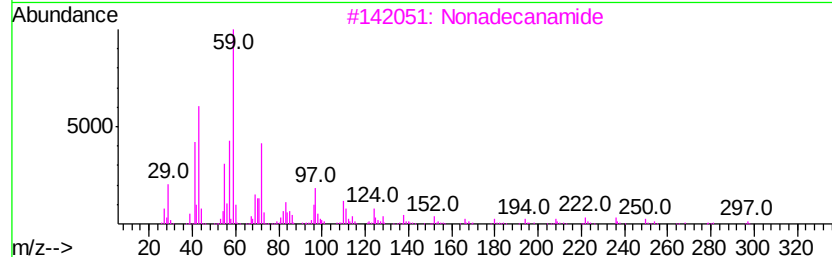
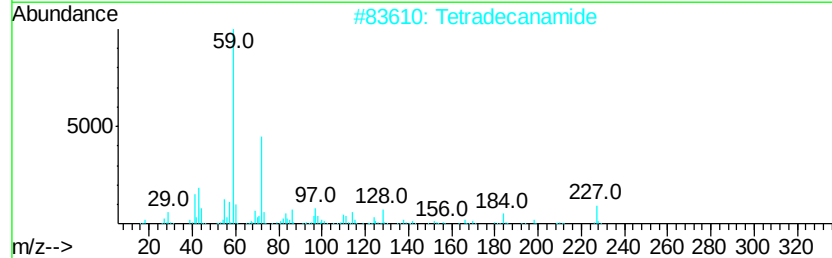
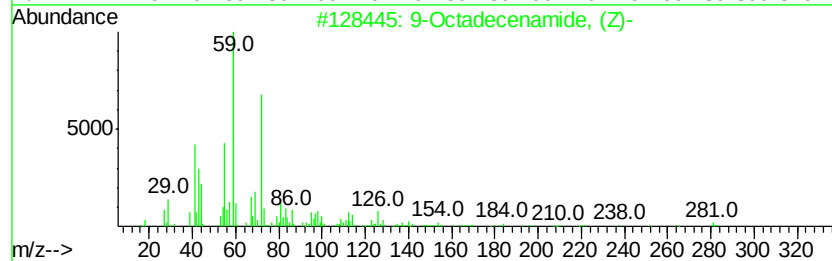
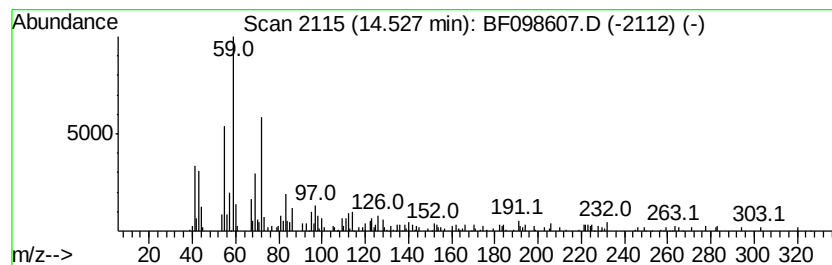
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	4.47 ng	137834	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Nonadecanamide	297	C19H39NO	058185-32-3	50
4		trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	38
5		2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	35



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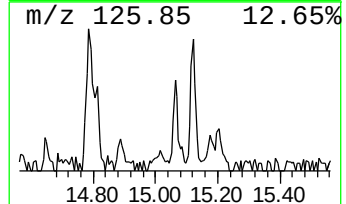
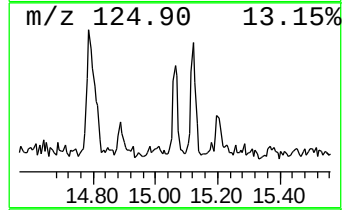
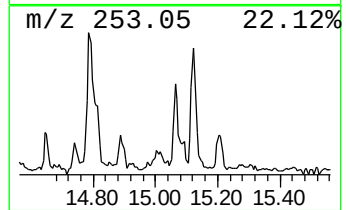
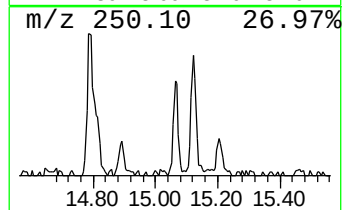
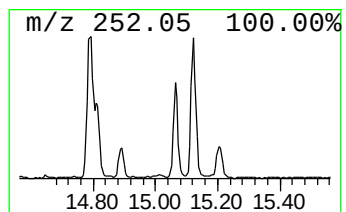
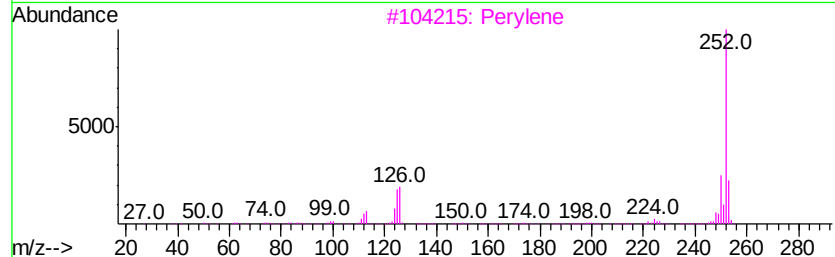
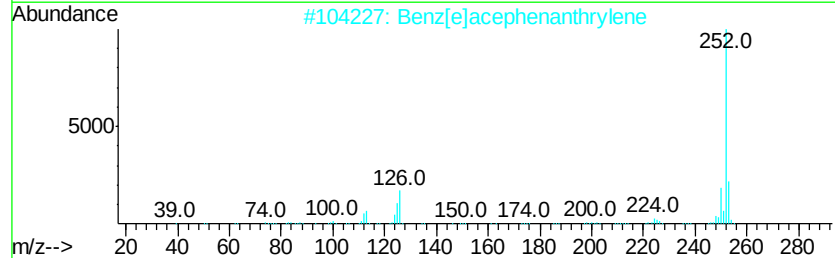
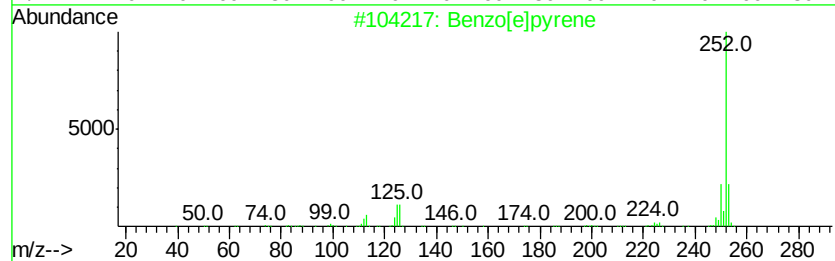
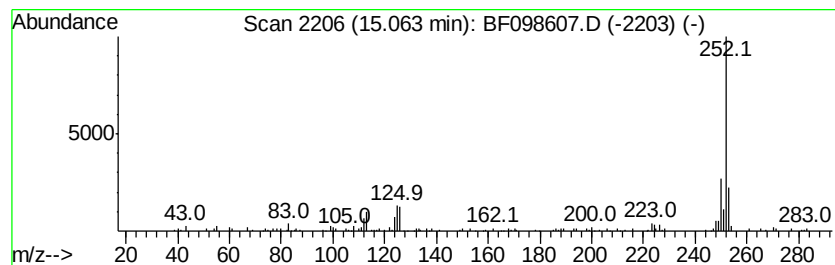
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.08 ng	94980	Perylene-d12	15.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3		Perylene	252	C20H12	000198-55-0	94
4		Benzo[a]pyrene	252	C20H12	000050-32-8	94
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\
Data File : BF098607.D
Acq On : 18 Sep 2017 17:36
Operator : SJ/JU
Sample : I5244-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

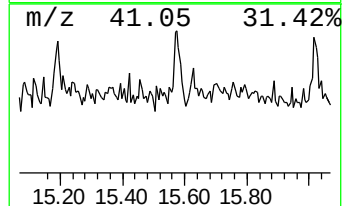
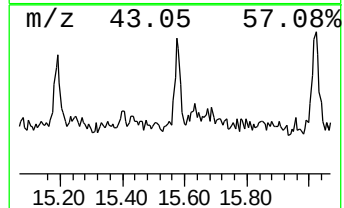
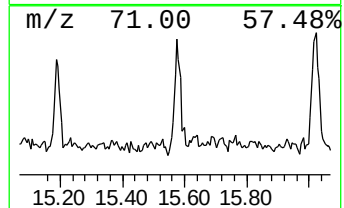
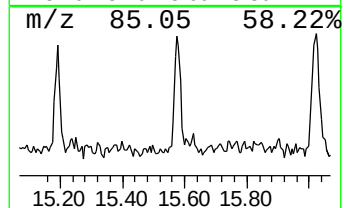
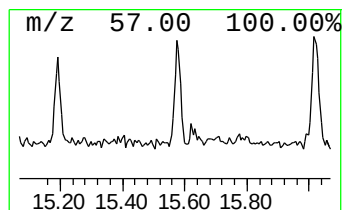
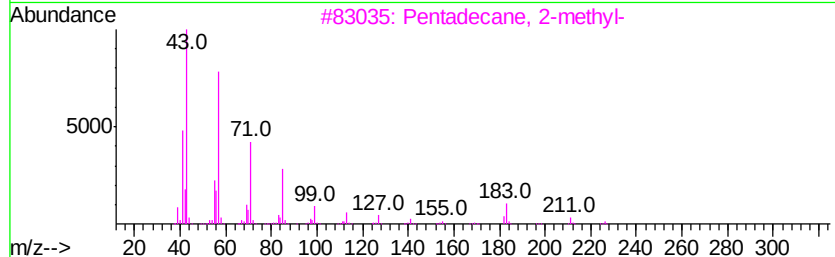
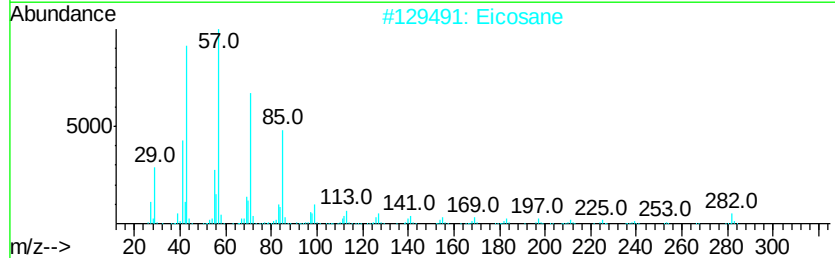
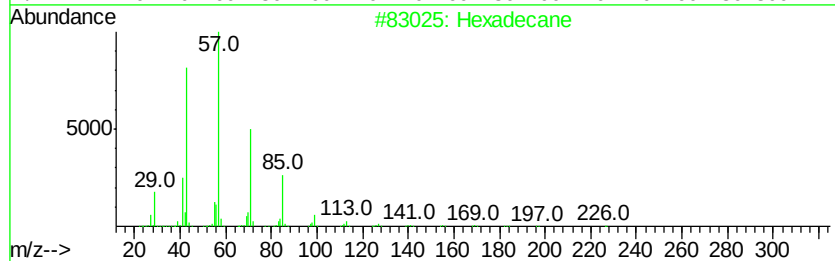
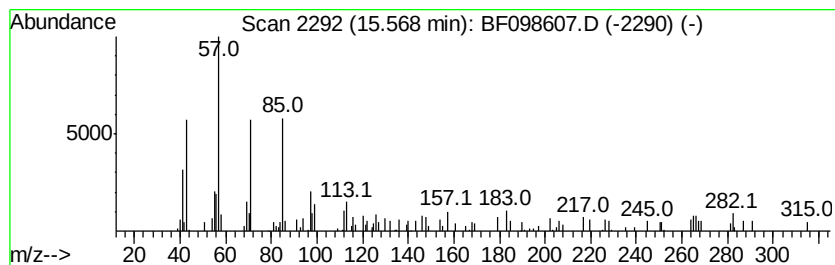
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ClientSampleId :
SASP2P-TP-106-X(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.57	2.51 ng	77482	Perylene-d12	15.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Eicosane	282	C20H42	000112-95-8	70
3	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	58
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58
5	Octacosane	394	C28H58	000630-02-4	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
Data File : BF098607.D
Acq On : 18 Sep 2017 17:36
Operator : SJ/JU
Sample : I5244-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-X(0-5)COMP

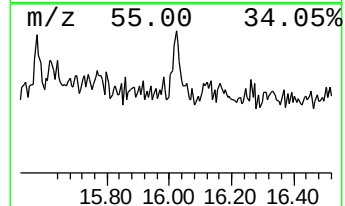
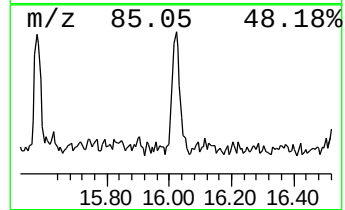
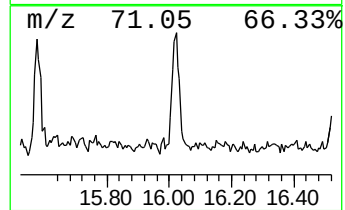
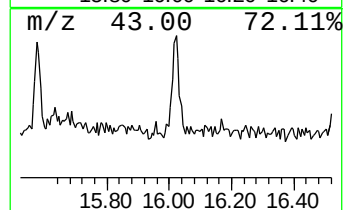
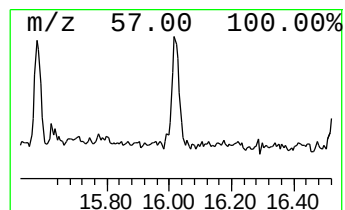
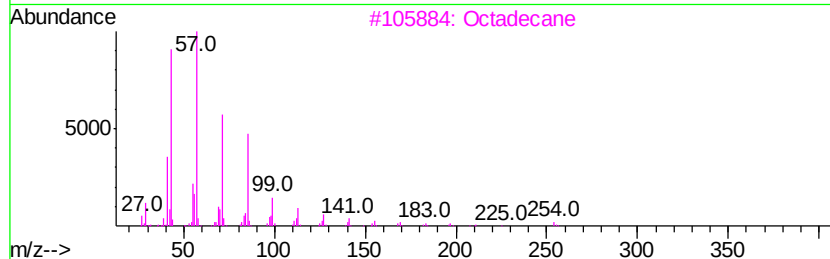
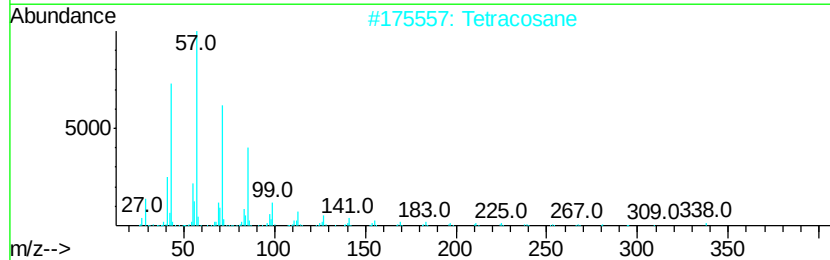
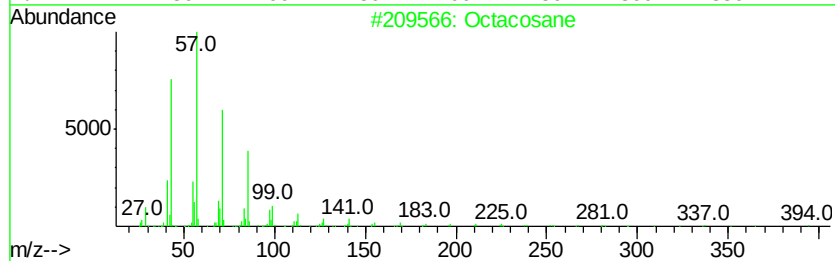
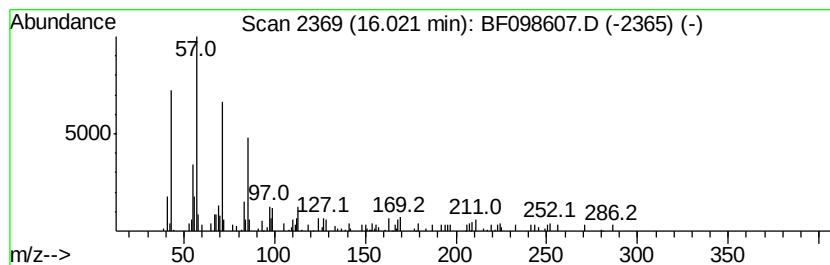
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.04 ng	93777	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Tetracosane	338	C24H50	000646-31-1	83
3		Octadecane	254	C18H38	000593-45-3	83
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5		Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
Data File : BF098607.D
Acq On : 18 Sep 2017 17:36
Operator : SJ/JU
Sample : I5244-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-X(0-5)COMP

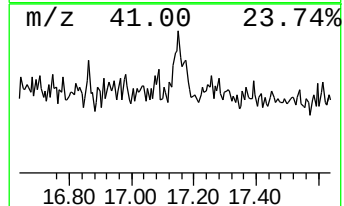
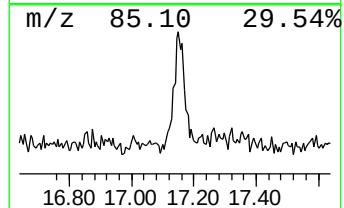
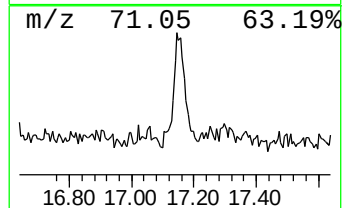
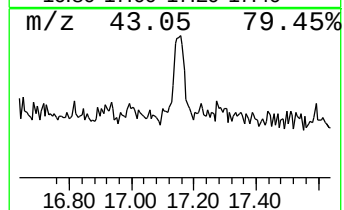
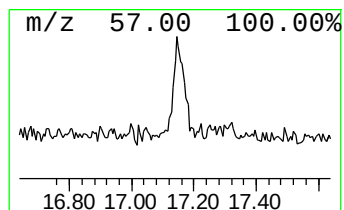
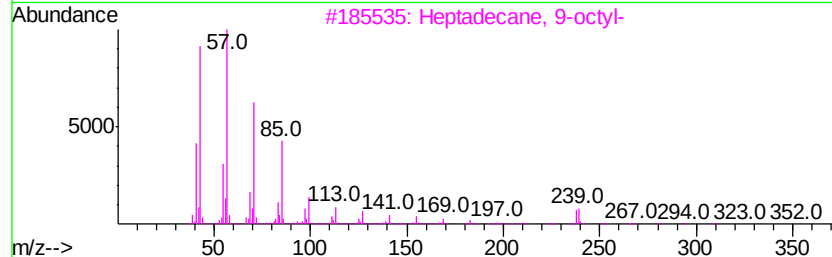
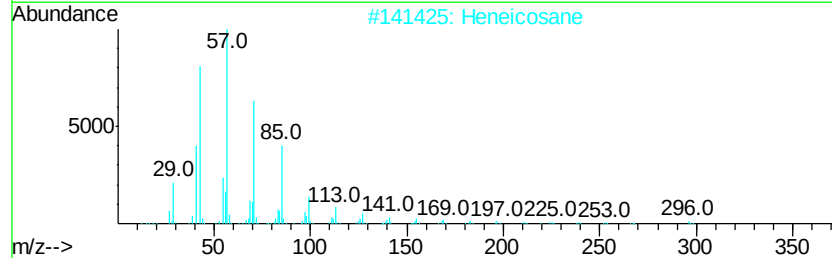
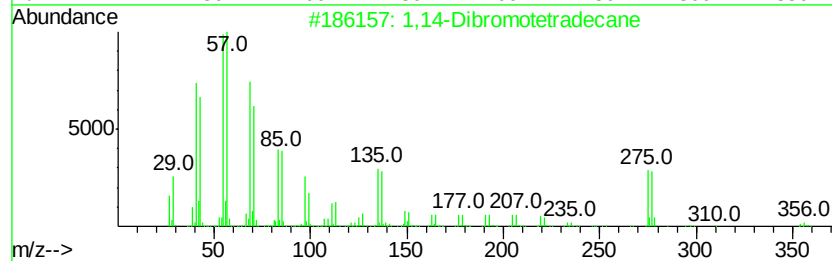
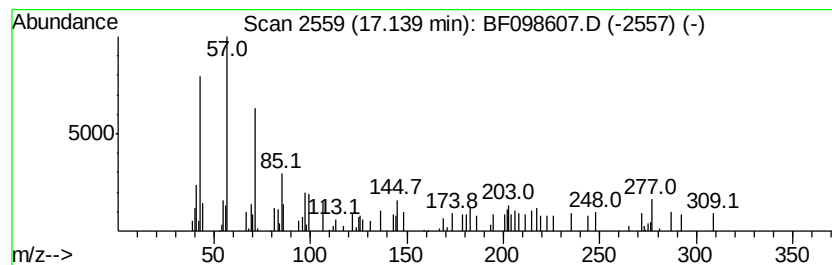
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.14 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	2.95 ng	90991	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,14-Dibromotetradecane	354	C14H28Br2	037688-96-3	14
2		Heneicosane	296	C21H44	000629-94-7	10
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	10
4		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	10
5		Heptacosane	380	C27H56	000593-49-7	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
Data File : BF098607.D
Acq On : 18 Sep 2017 17:36
Operator : SJ/JU
Sample : I5244-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-TP-106-X(0-5)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.82	10.2	ng	351278	1	6.63	687890	20.0
unknown6.41	6.41	98.7	ng	3394100	1	6.63	687890	20.0
Trichloroacetic a...	13.63	4.1	ng	169883	5	13.78	826958	20.0
9-Octadecenamide,...	14.53	4.5	ng	137834	6	15.18	616229	20.0
Benzo[e]pyrene	15.06	3.1	ng	94980	6	15.18	616229	20.0
Hexadecane	15.57	2.5	ng	77482	6	15.18	616229	20.0
Octacosane	16.02	3.0	ng	93777	6	15.18	616229	20.0
unknown17.14	17.14	3.0	ng	90991	6	15.18	616229	20.0