

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
 Data File : BG033679.D
 Acq On : 9 Apr 2018 14:08
 Operator : SJ/JU
 Sample : J2227-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-1

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

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.475	26	32	43	rBV	65618	140930	4.09%	0.968%
2	3.569	43	48	57	rVB	52469	87407	2.54%	0.601%
3	5.773	414	423	431	rBV	40901	74206	2.15%	0.510%
4	6.284	503	510	536	rBV	685843	1334004	38.70%	9.166%
5	7.970	790	797	818	rBV	678609	1470095	42.65%	10.101%
6	8.370	857	865	888	rBV	652966	1368632	39.71%	9.404%
7	9.192	996	1005	1021	rBV	497171	1011529	29.35%	6.950%
8	10.056	1144	1152	1173	rBV2	368488	881693	25.58%	6.058%
9	14.104	1833	1841	1856	rBV	1117076	1954771	56.72%	13.432%
10	14.891	1968	1975	1984	rBV	72951	127115	3.69%	0.873%
11	16.237	2201	2204	2210	rVB	37155	46034	1.34%	0.316%
12	16.948	2318	2325	2343	rBV	1125929	1844956	53.53%	12.677%
13	17.095	2345	2350	2360	rVB	34589	68649	1.99%	0.472%
14	19.004	2669	2675	2684	rBV2	74581	125558	3.64%	0.863%
15	20.726	2962	2968	2979	rBV	2621447	3446618	100.00%	23.682%
16	22.065	3191	3196	3202	rBV7	19681	38140	1.11%	0.262%
17	23.828	3488	3496	3504	rBV4	69944	156575	4.54%	1.076%
18	24.415	3588	3596	3607	rVB2	171580	376632	10.93%	2.588%

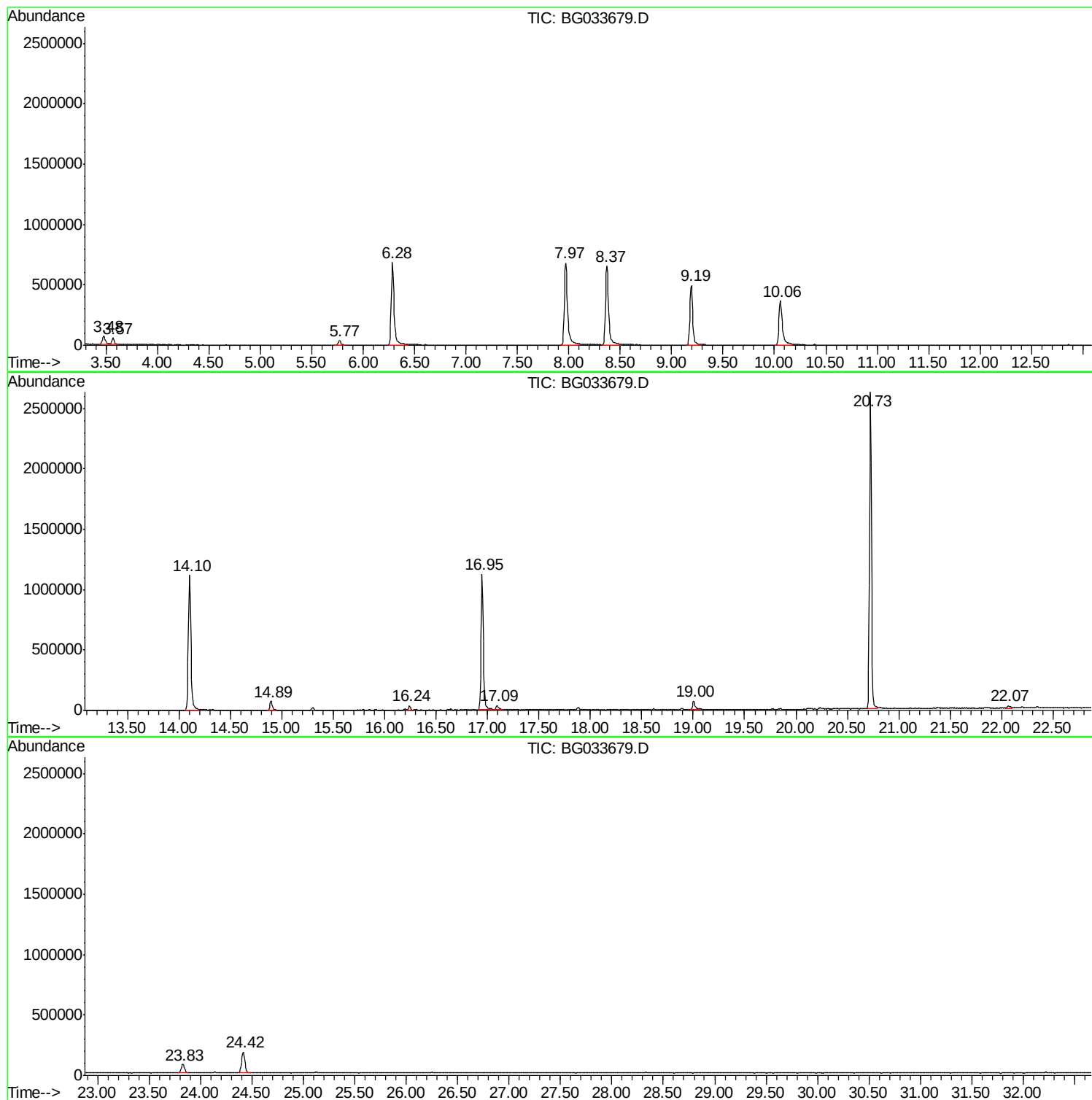
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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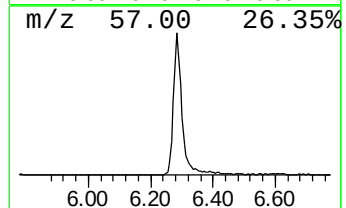
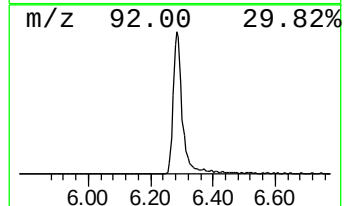
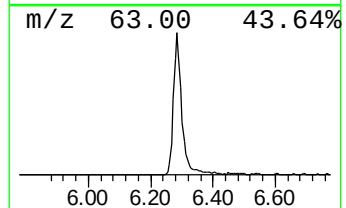
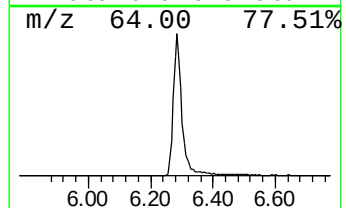
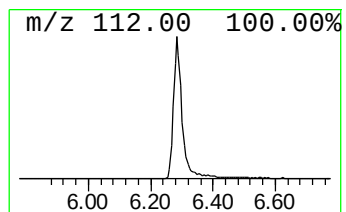
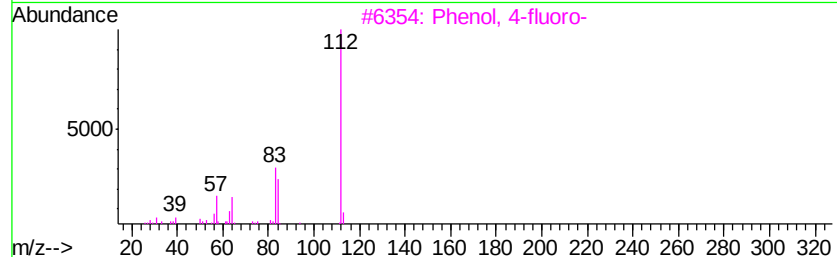
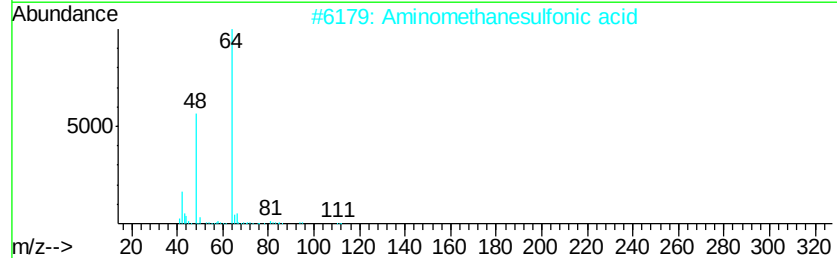
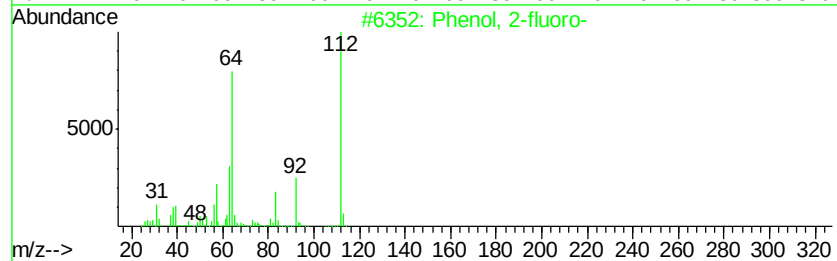
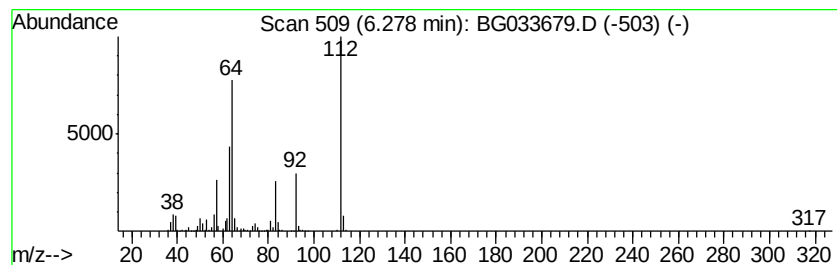
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenol, 2-fluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.28	30.26 ng	1334000	Napthalene-d8	11.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 2-fluoro-	112 C6H5FO	000367-12-4	93
2	Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9	23
3	Phenol, 4-fluoro-	112 C6H5FO	000371-41-5	10
4	2-Aminoethyl hydrogen sulfate	141 C2H7NO4S	000926-39-6	9
5	Ethyl Chloride	64 C2H5Cl	000075-00-3	7



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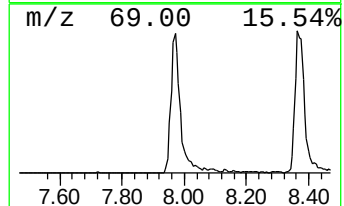
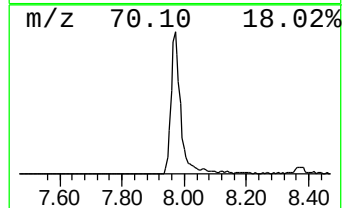
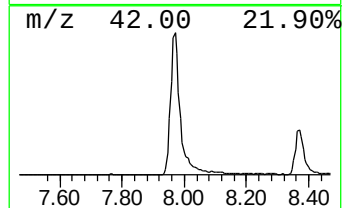
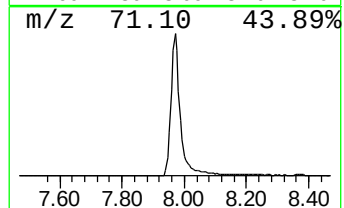
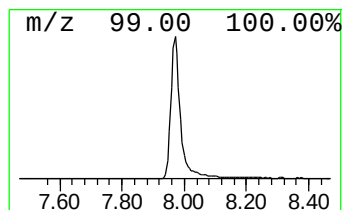
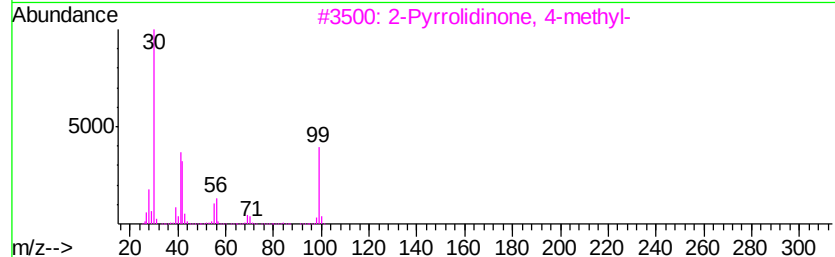
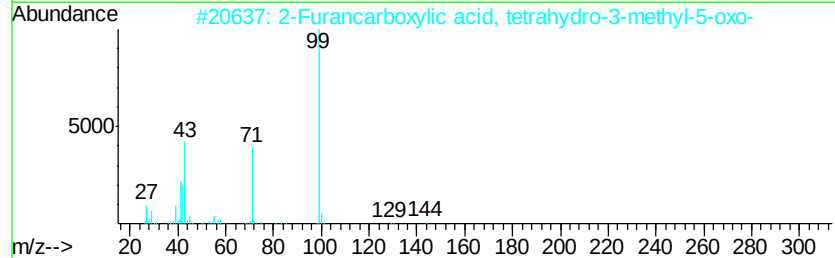
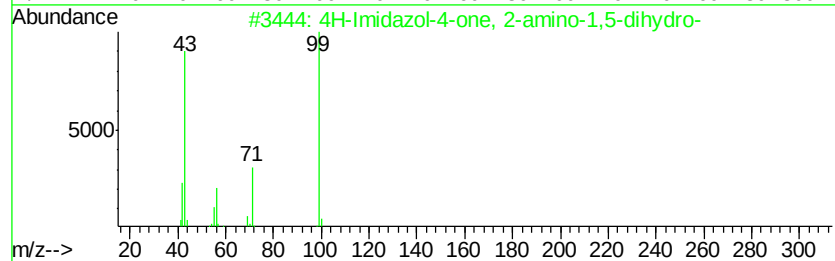
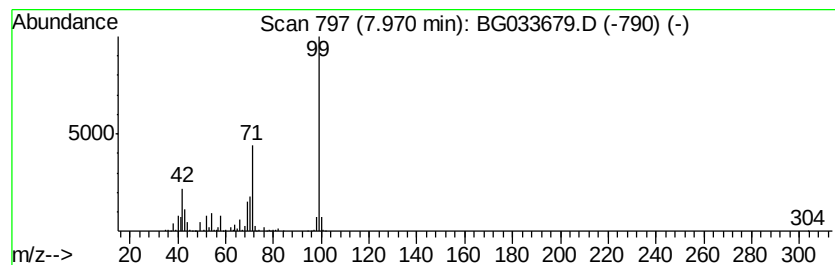
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Peak Number 3 4H-Imidazol-4-one, 2-amino-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	33.35 ng	1470100	Naphthalene-d8	11.58

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	64
2		2-Furancarboxylic acid, tetrahyd...	144	C6H8O4	022073-04-7	45
3		2-Pyrrolidinone, 4-methyl-	99	C5H9NO	1000197-00-3	43
4		3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
5		Phenol-d6-	100	C6D6O	013127-88-3	40



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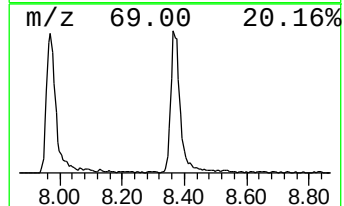
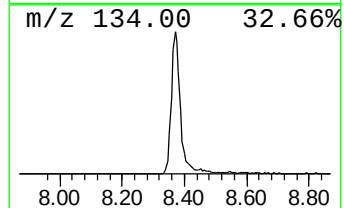
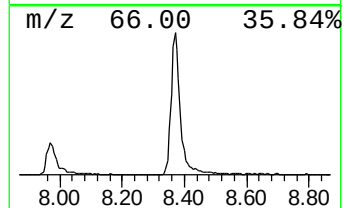
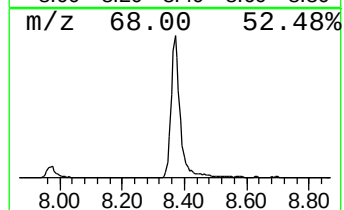
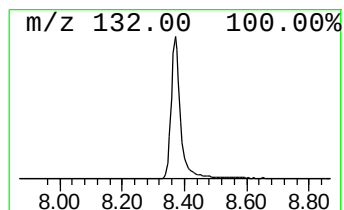
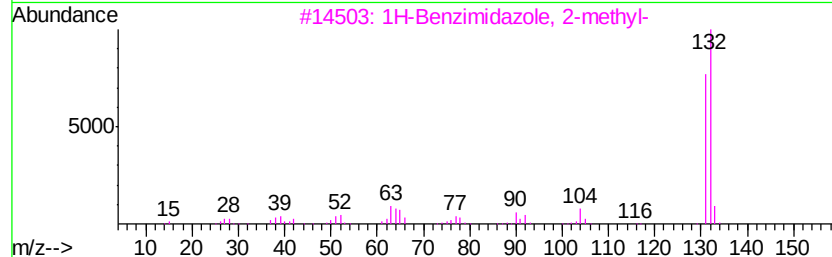
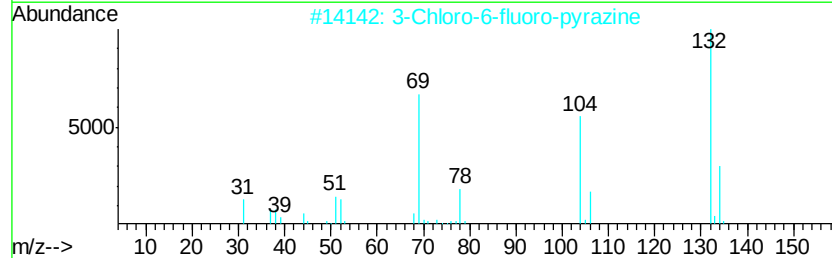
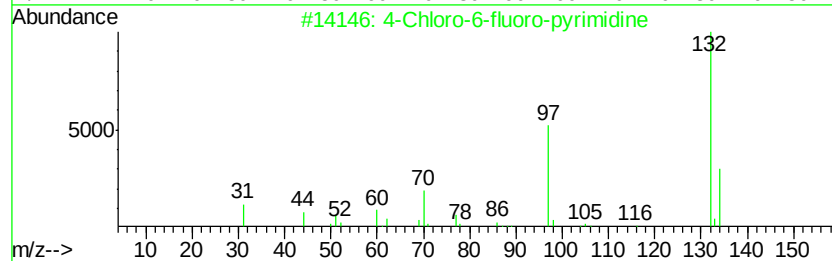
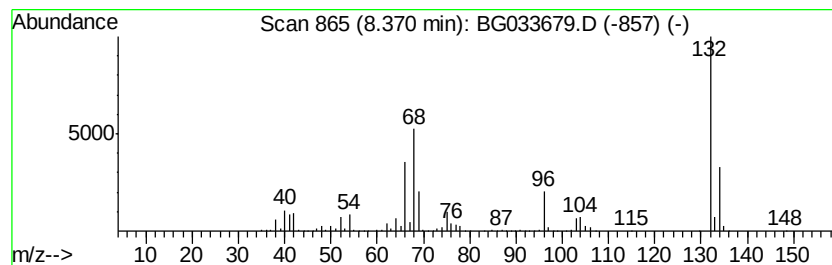
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Peak Number 4 unknown8.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	31.05 ng	1368630	Napthalene-d8	11.58

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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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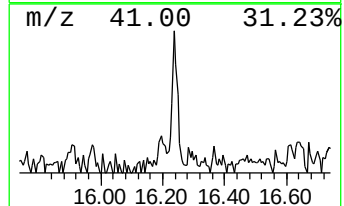
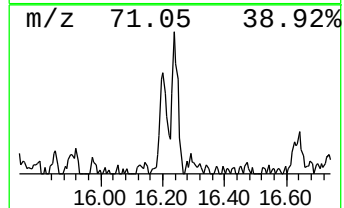
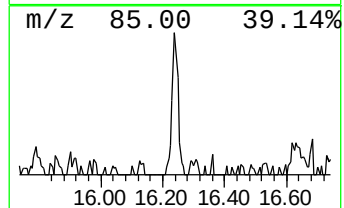
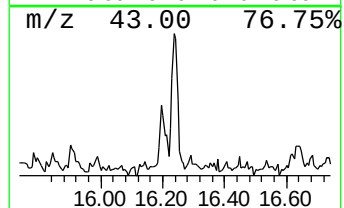
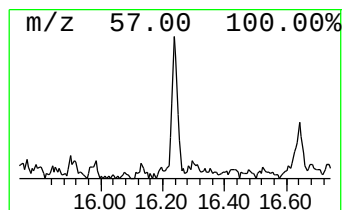
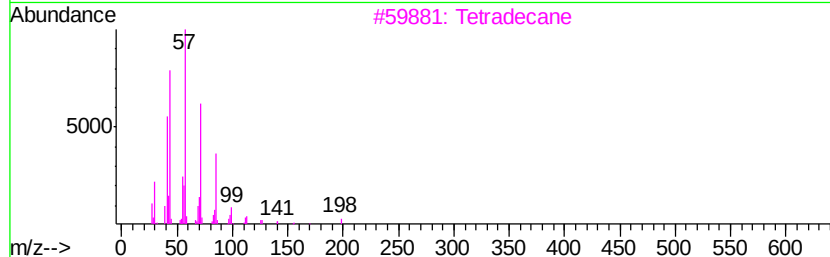
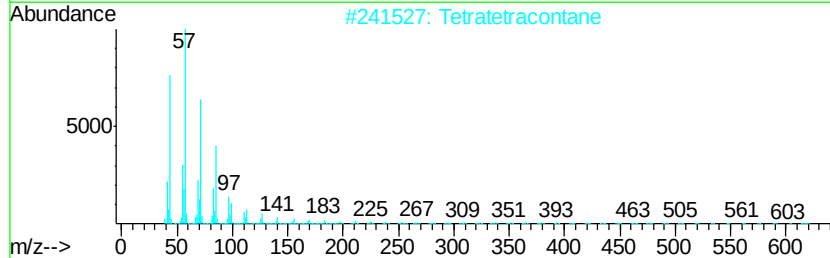
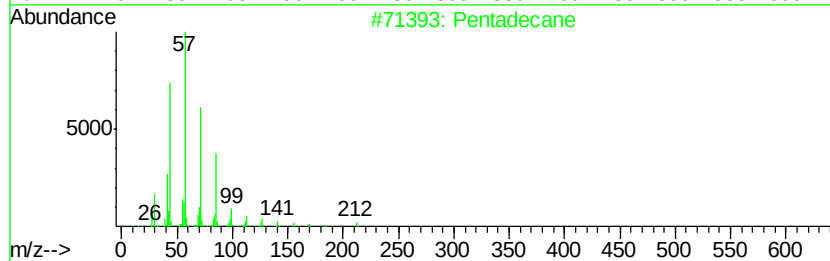
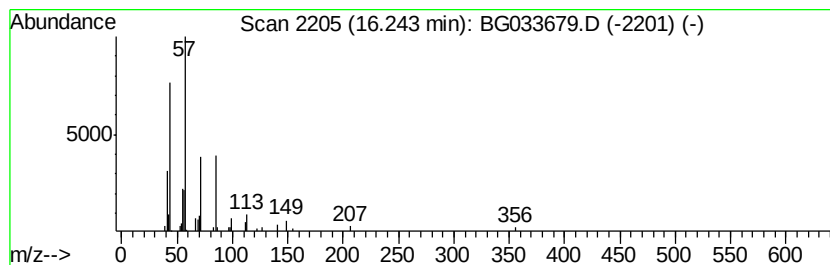
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	13.41 ng	46034	Phenanthrene-d10	17.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Tetratetracontane		619	C44H90	007098-22-8	90
3	Tetradecane		198	C14H30	000629-59-4	86
4	Heptacosane		380	C27H56	000593-49-7	78
5	Hexadecane		226	C16H34	000544-76-3	78



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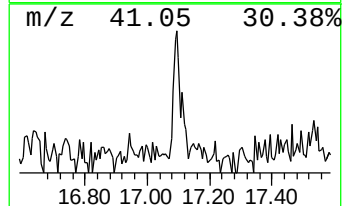
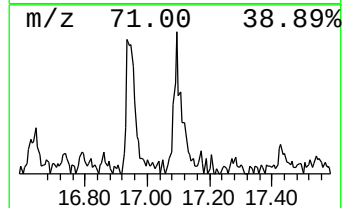
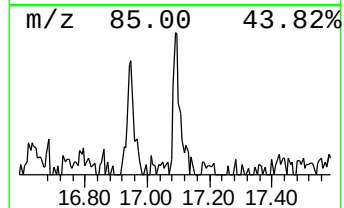
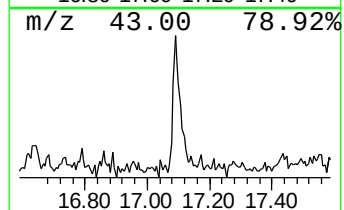
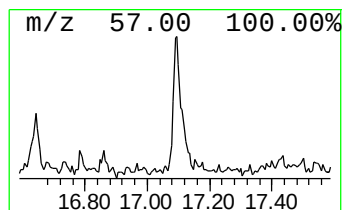
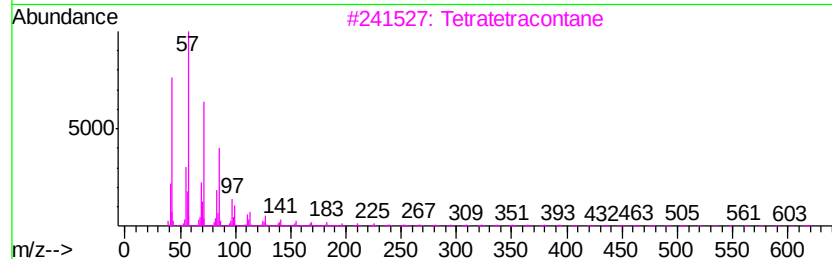
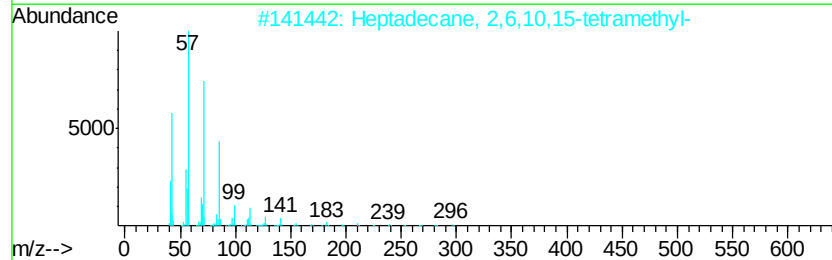
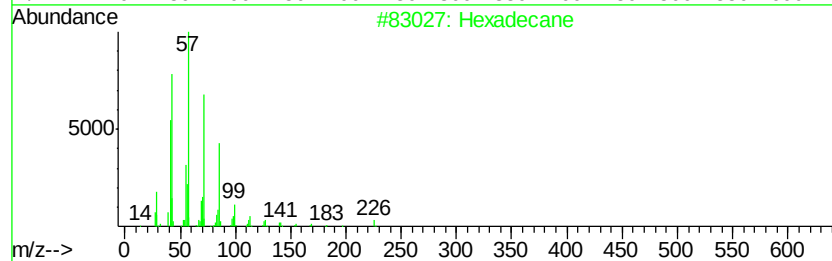
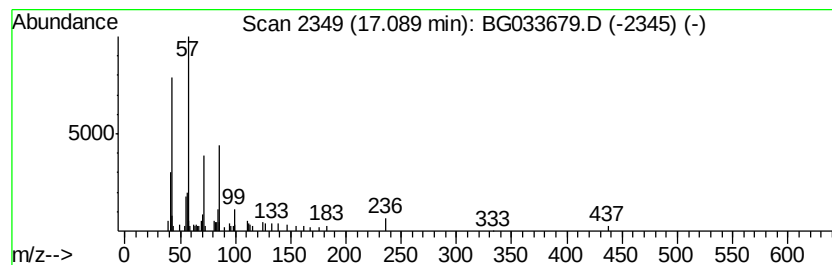
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Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.09	20.00 ng	68649	Phenanthrene-d10		17.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	87
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	86
3	Tetratetracontane		619	C44H90	007098-22-8	86
4	Pentadecane		212	C15H32	000629-62-9	80
5	10-Methylnonadecane		282	C20H42	056862-62-5	80



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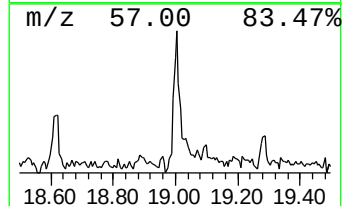
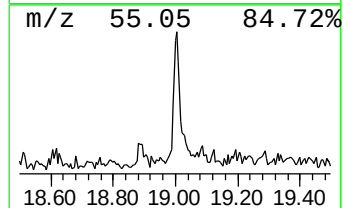
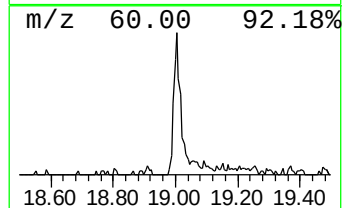
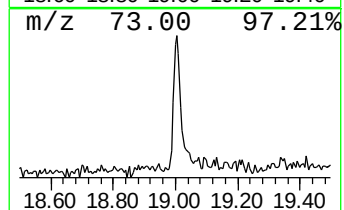
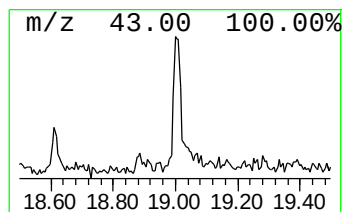
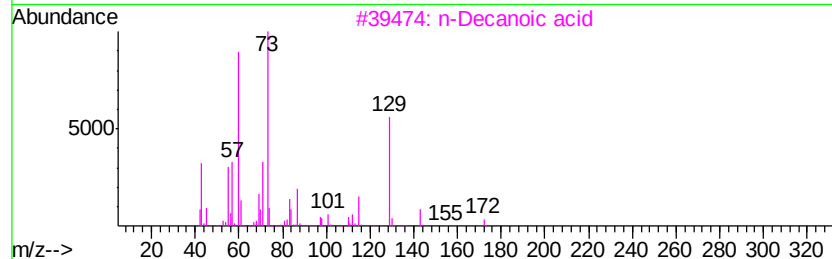
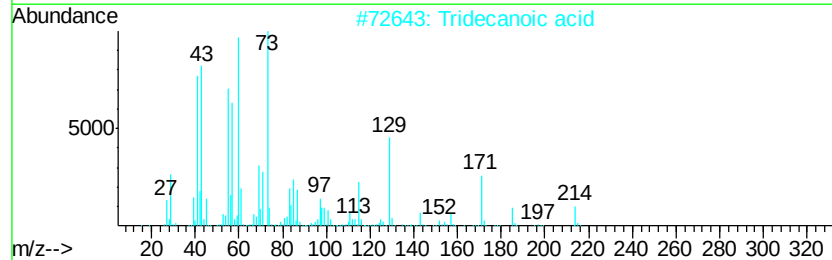
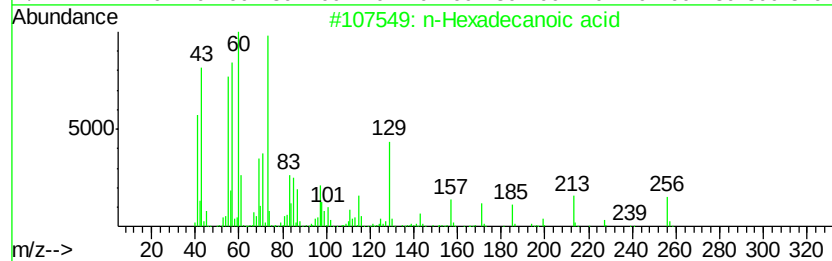
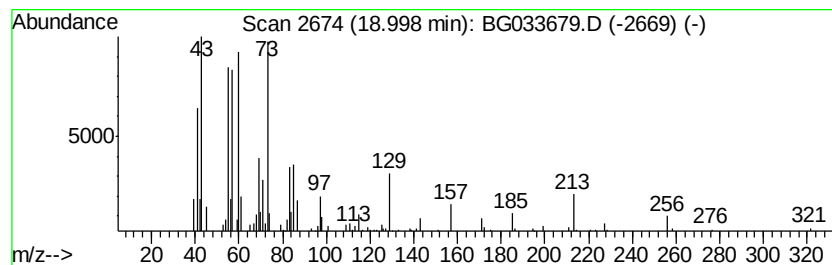
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.00	36.58 ng	125558	Phenanthrene-d10		17.43
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033679.D
Acq On : 9 Apr 2018 14:08
Operator : SJ/JU
Sample : J2227-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

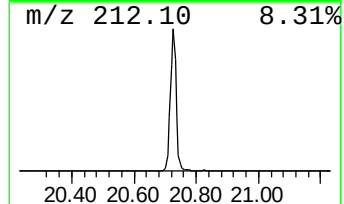
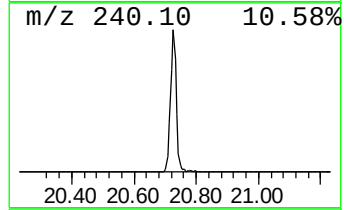
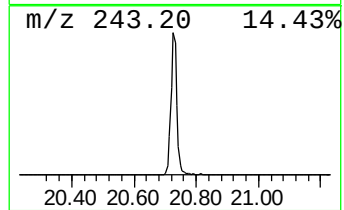
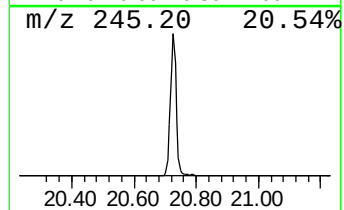
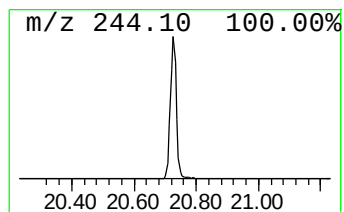
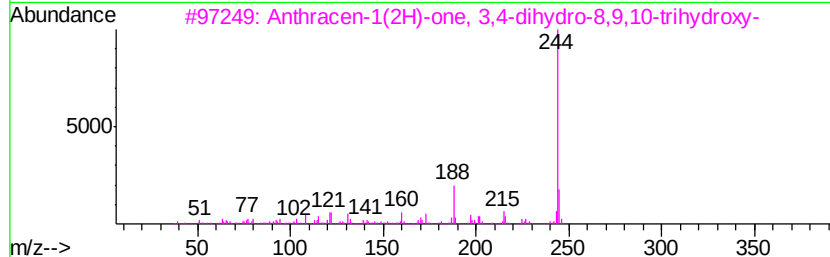
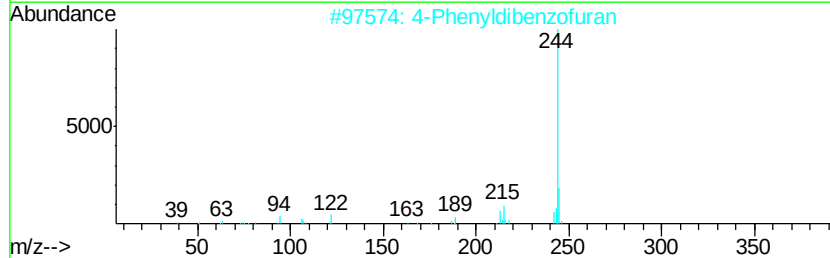
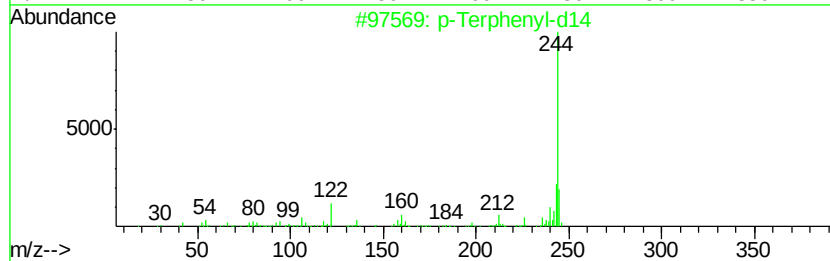
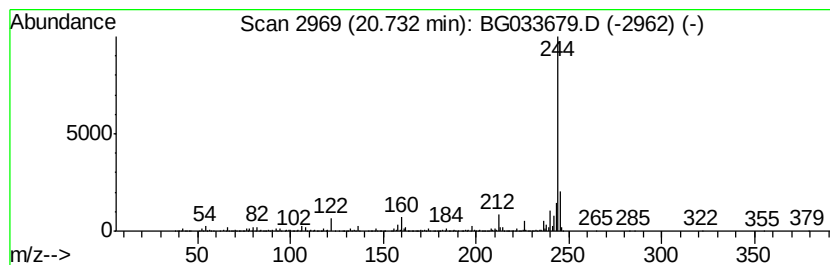
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 p-Terphenyl-d14 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	1807.35 ng	3446620	Chrysene-d12	21.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	p-Terphenyl-d14	244	C18D14	001718-51-0	90
2		4-Phenyldibenzofuran	244	C18H12O	1000314-39-5	74
3		Anthracen-1(2H)-one, 3,4-dihydro...	244	C14H12O4	037802-95-2	64
4		Imidazo[1,2-a]pyridine, 2-(2-nap...	244	C17H12N2	038922-71-3	64
5		4-Benzylbiphenyl	244	C19H16	000613-42-3	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
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Acq On : 9 Apr 2018 14:08
Operator : SJ/JU
Sample : J2227-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

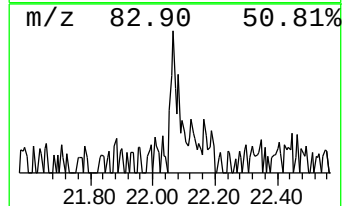
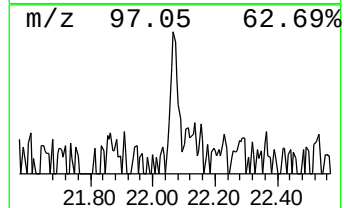
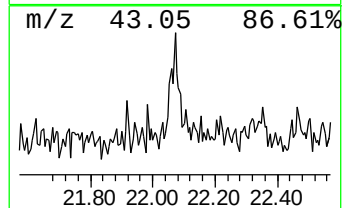
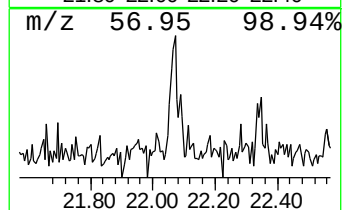
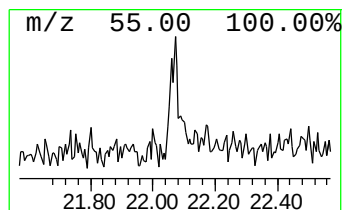
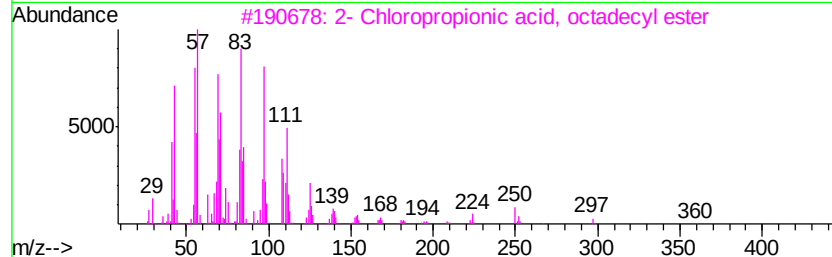
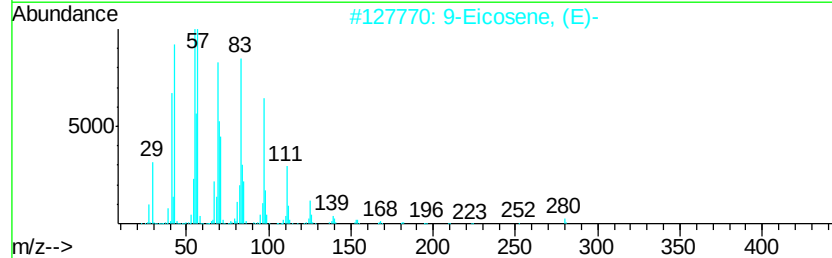
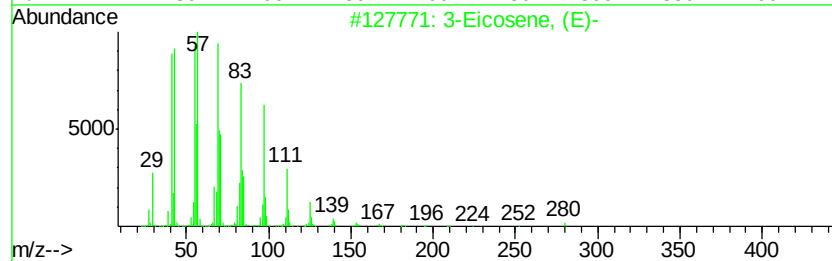
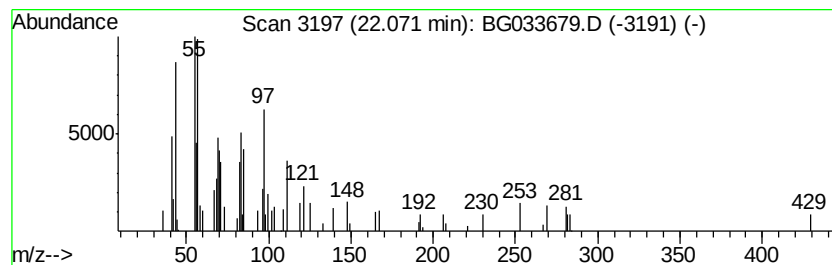
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	20.00 ng	38140	Chrysene-d12	21.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	89
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	86
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	58
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	49



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033679.D
Acq On : 9 Apr 2018 14:08
Operator : SJ/JU
Sample : J2227-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

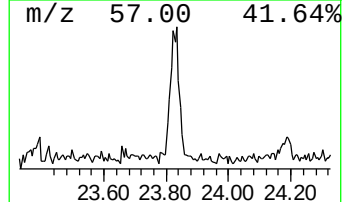
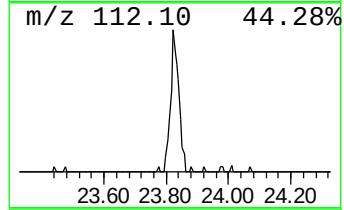
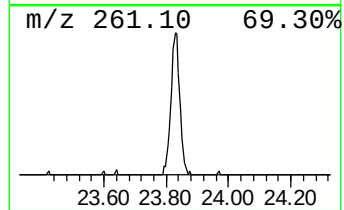
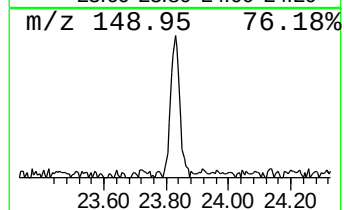
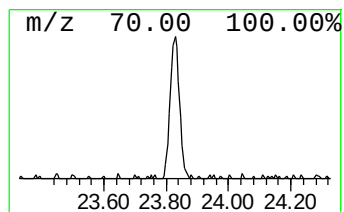
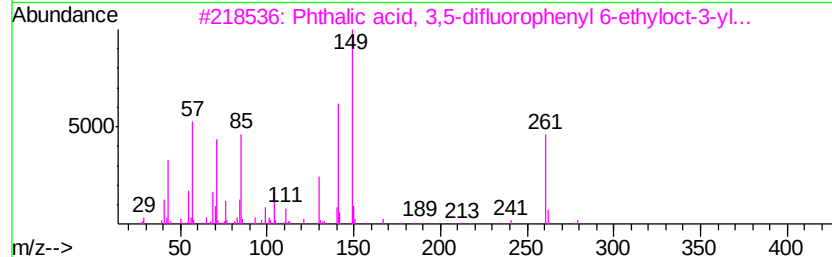
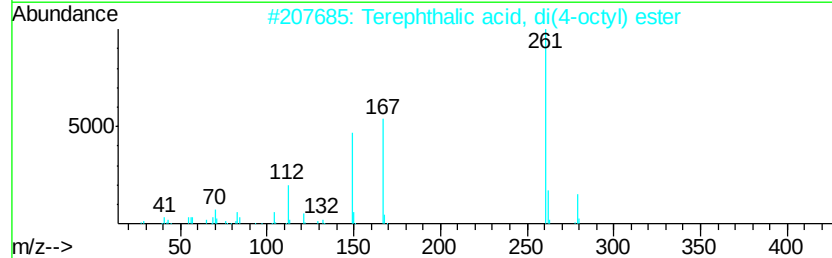
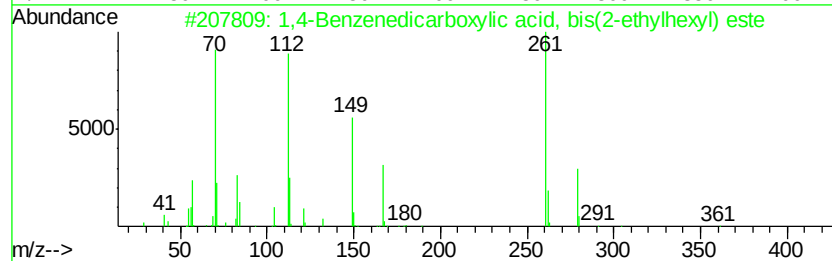
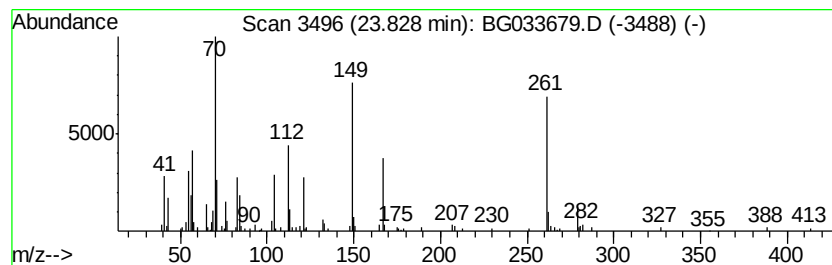
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown23.83 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.83	8.31 ng	156575	Perylene-d12	25.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	47
2		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	35
3		Phthalic acid, 3,5-difluoropheny...	418	C24H28F2O4	1000315-53-1	27
4		9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	27
5		Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033679.D
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Sample : J2227-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

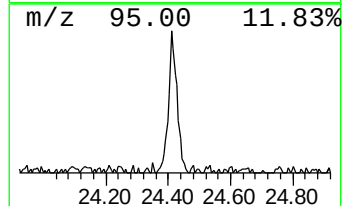
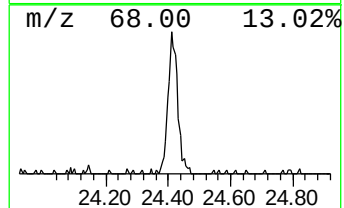
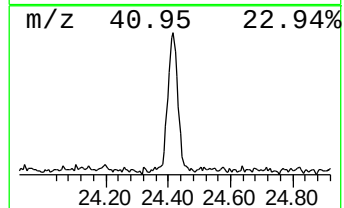
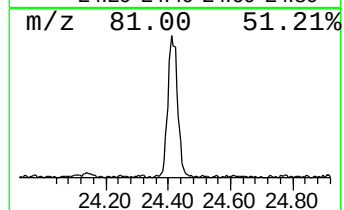
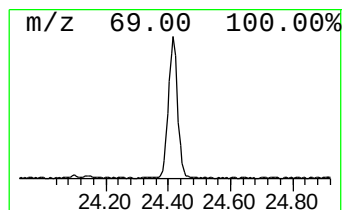
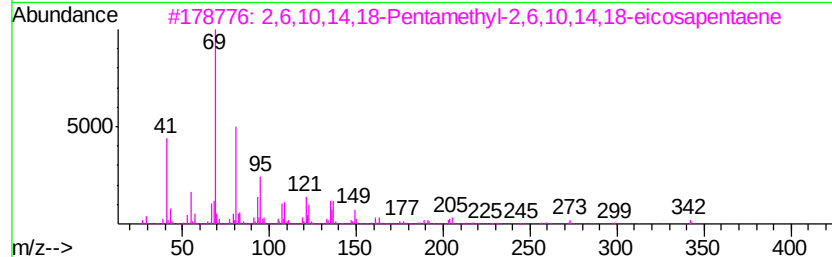
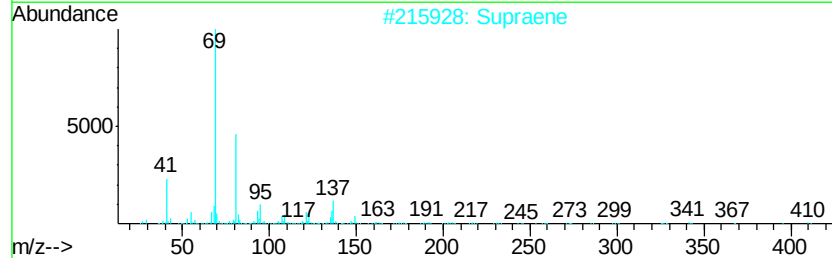
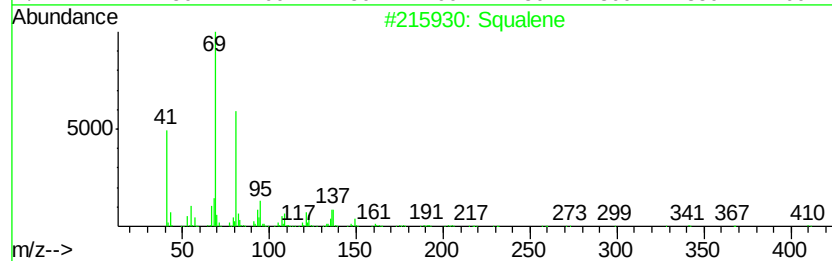
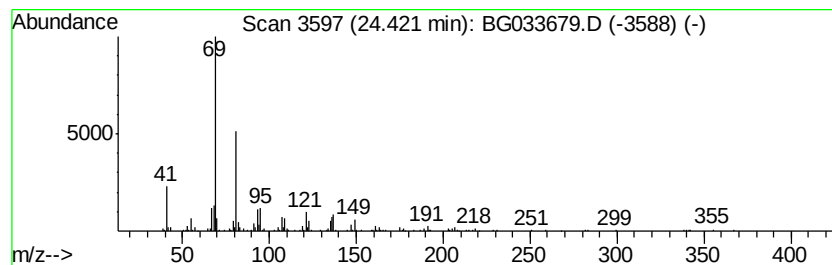
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.42	20.00 ng	376632	Perylene-d12	25.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	91
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342 C25H42	075581-03-2	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547 C40H66	000502-62-5	83
5	trans-Farnesol	222 C15H26O	000106-28-5	78



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040918\
 Data File : BG033679.D
 Acq On : 9 Apr 2018 14:08
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 Sample : J2227-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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
Phenol, 2-fluoro-	6.28	30.3	ng	1334000	1	11.58	881693	20.0
4H-Imidazol-4-one...	7.97	33.4	ng	1470100	1	11.58	881693	20.0
unknown8.37	8.37	31.1	ng	1368630	1	11.58	881693	20.0
Pentadecane	16.24	13.4	ng	46034	3	17.43	68649	20.0
Hexadecane	17.09	20.0	ng	68649	3	17.43	68649	20.0
n-Hexadecanoic acid	19.00	36.6	ng	125558	3	17.43	68649	20.0
p-Terphenyl-d14	20.73	1807.3	ng	3446620	4	21.50	38140	20.0
3-Eicosene, (E)-	22.07	20.0	ng	38140	4	21.50	38140	20.0
unknown23.83	23.83	8.3	ng	156575	5	25.06	376632	20.0
Squalene	24.42	20.0	ng	376632	5	25.06	376632	20.0