

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG016981.D
 Acq On : 9 May 2015 7:39
 Operator : TP/IZ
 Sample : G2058-07
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MPE-9

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_G\METHODS\8270-BG050515.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	2.914	33	38	47	rBV	288763	459985	9.20%	1.698%
2	2.990	47	51	62	rVB	573680	697608	13.95%	2.575%
3	4.912	372	378	383	rVB	45977	62816	1.26%	0.232%
4	5.376	450	457	466	rBV	486192	718639	14.37%	2.652%
5	6.956	720	726	735	rBV	346084	537252	10.75%	1.983%
6	7.321	780	788	798	rBV	979823	1573802	31.48%	5.808%
7	7.791	862	868	874	rBV	231794	351123	7.02%	1.296%
8	8.108	915	922	931	rVB	853169	1377570	27.55%	5.084%
9	8.948	1058	1065	1073	rBV	826034	1351442	27.03%	4.988%
10	10.581	1333	1343	1350	rBV	326153	556158	11.12%	2.053%
11	13.049	1756	1763	1771	rBV	2079330	3015655	60.32%	11.129%
12	14.430	1991	1998	2005	rBV2	529855	809929	16.20%	2.989%
13	14.871	2063	2073	2087	rBV	763478	1361053	27.22%	5.023%
14	15.916	2244	2251	2266	rBV	1933608	2680658	53.62%	9.893%
15	17.168	2458	2464	2470	rBV2	723337	1050412	21.01%	3.877%
16	17.937	2589	2595	2602	rBV7	42641	75458	1.51%	0.278%
17	18.067	2612	2617	2626	rBV	199877	290083	5.80%	1.071%
18	18.496	2686	2690	2696	rVB2	55276	63633	1.27%	0.235%
19	19.224	2808	2814	2823	rBV2	32930	75222	1.50%	0.278%
20	19.348	2831	2835	2845	rBV2	85685	137014	2.74%	0.506%
21	19.800	2906	2912	2920	rVB	4046327	4999817	100.00%	18.452%
22	21.057	3121	3126	3131	rBV	121850	150181	3.00%	0.554%
23	21.263	3156	3161	3169	rBV	192841	231438	4.63%	0.854%
24	21.345	3169	3175	3186	rVV	883015	1193464	23.87%	4.405%
25	21.721	3236	3239	3247	rBV6	34091	54212	1.08%	0.200%
26	22.503	3366	3372	3376	rBV	583671	854923	17.10%	3.155%
27	22.544	3376	3379	3389	rVB	364880	518290	10.37%	1.913%
28	23.073	3464	3469	3473	rBV2	79653	127557	2.55%	0.471%
29	23.643	3558	3566	3574	rVB	550333	1089152	21.78%	4.020%
30	24.947	3780	3788	3803	rBV7	89437	331213	6.62%	1.222%
31	27.779	4260	4270	4281	rBV6	84936	300519	6.01%	1.109%

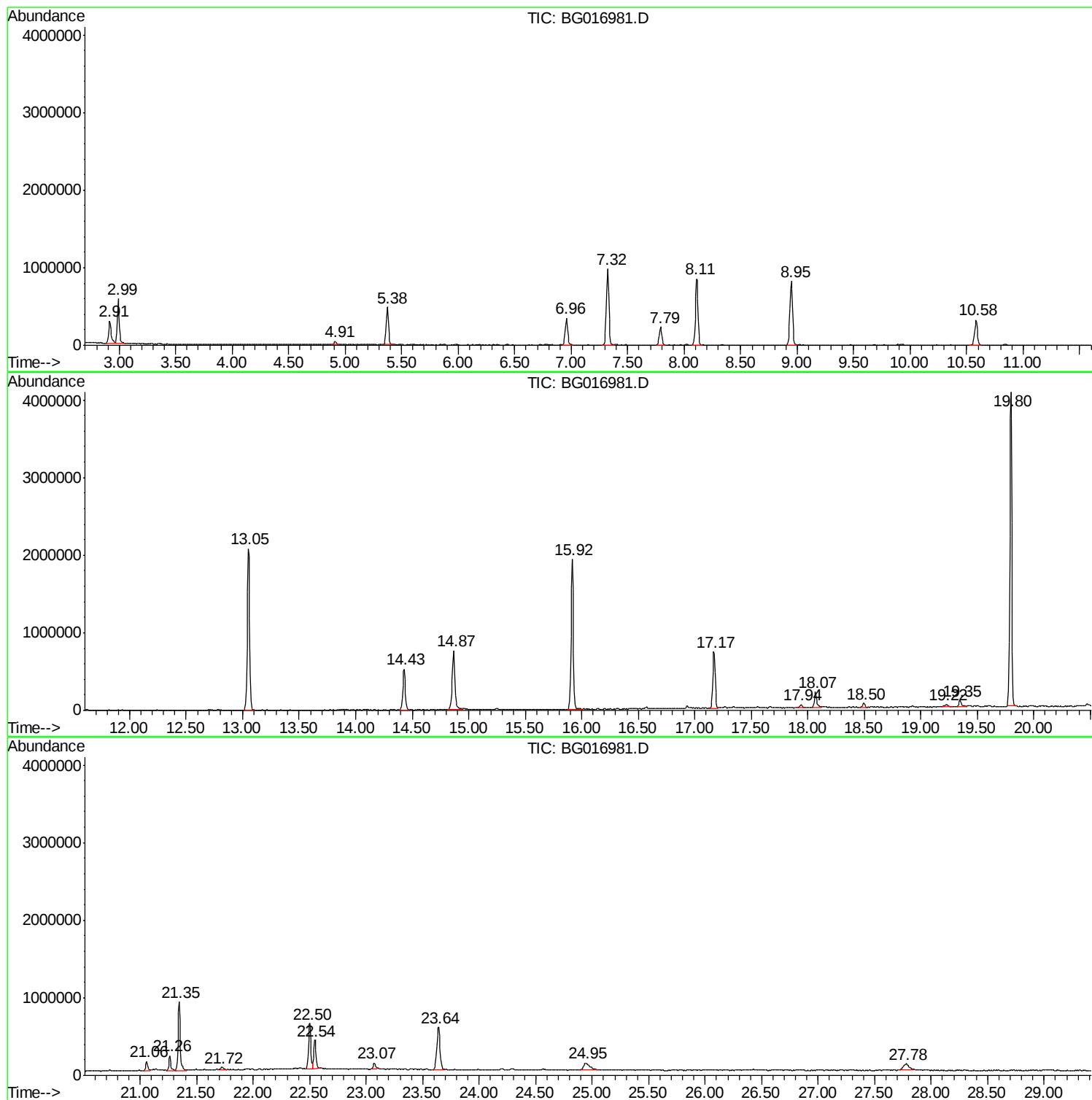
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Instrument :
BNA_G
ClientSampleId :
MPE-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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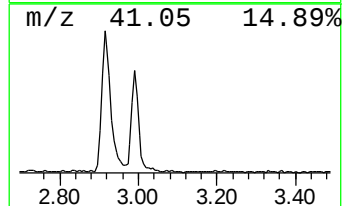
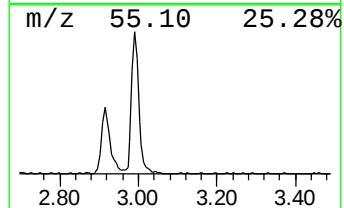
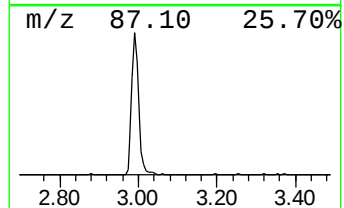
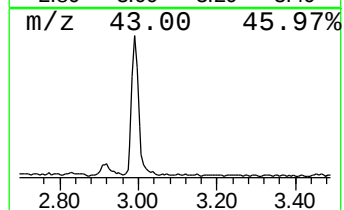
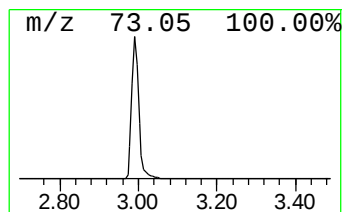
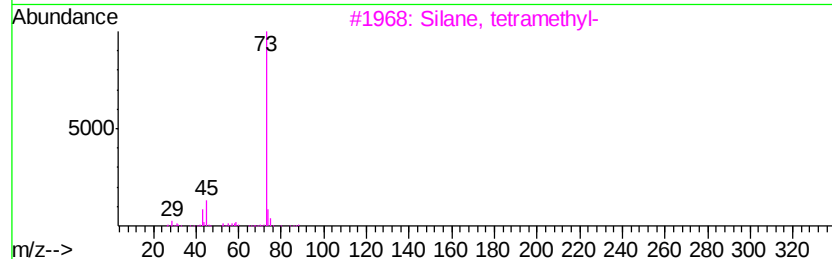
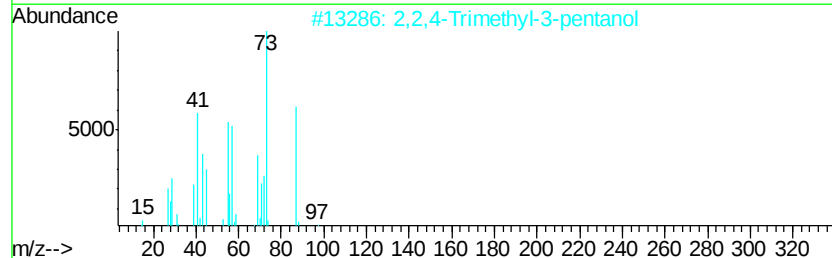
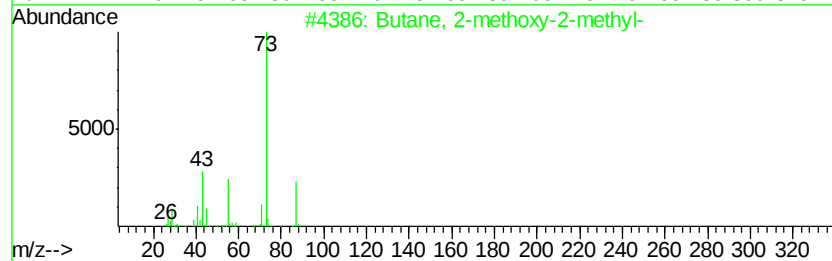
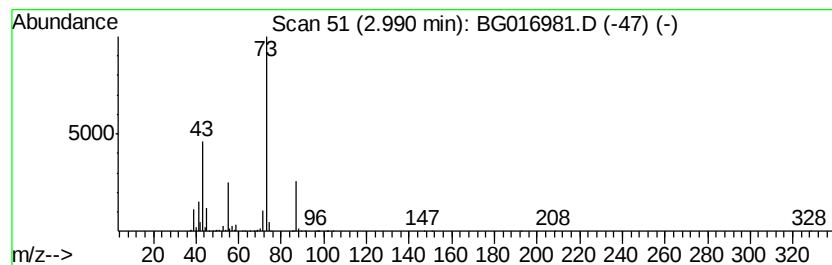
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	39.74 ng	697608	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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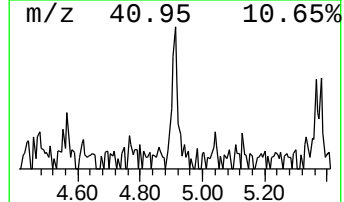
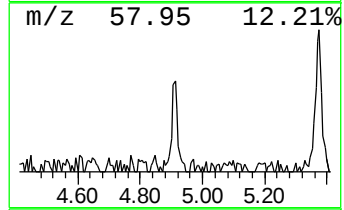
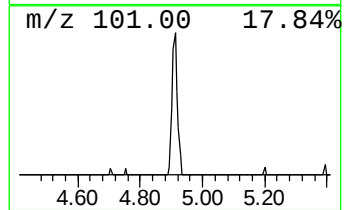
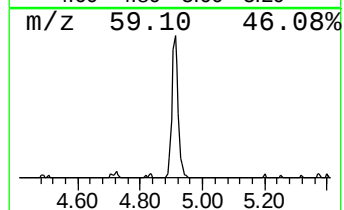
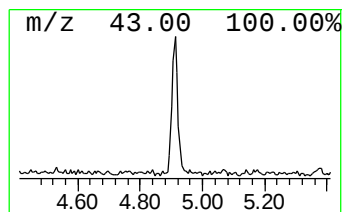
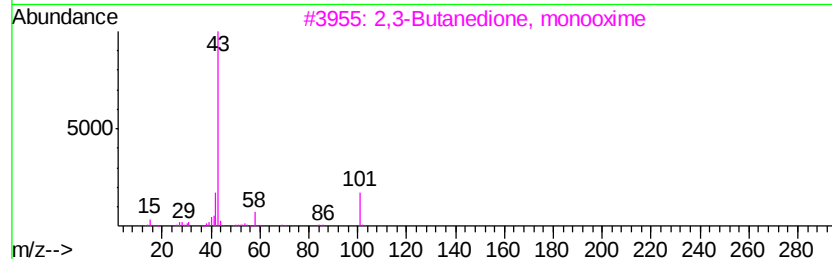
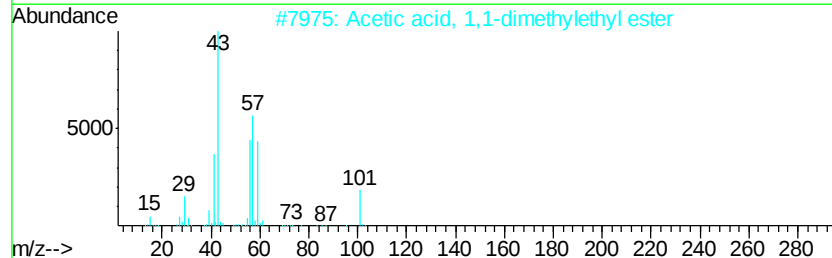
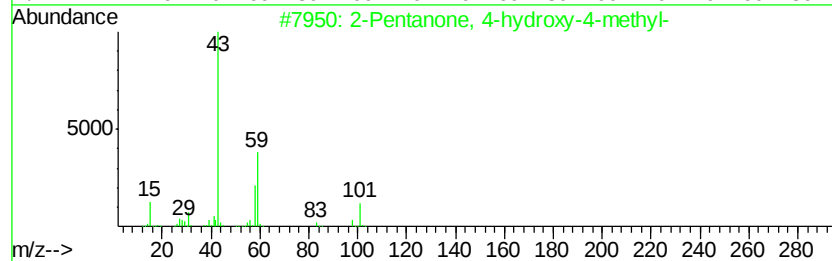
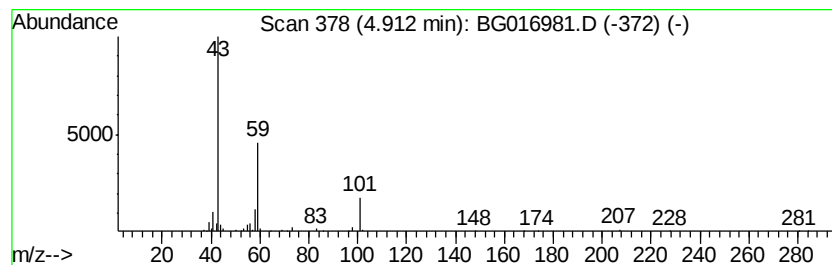
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown4.91 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.58 ng	62816	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Propylamine	59	C3H9N	000107-10-8	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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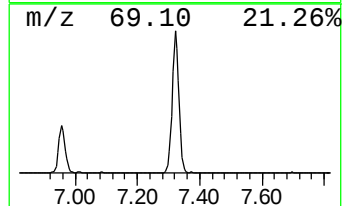
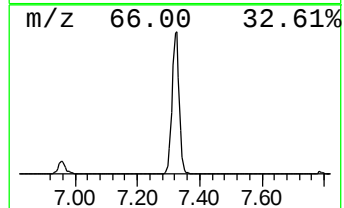
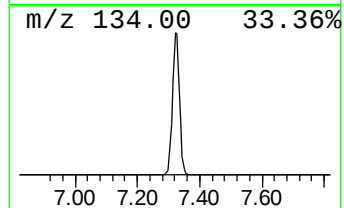
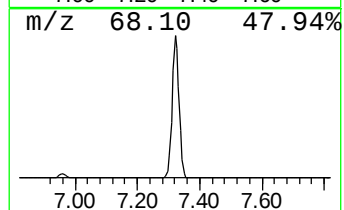
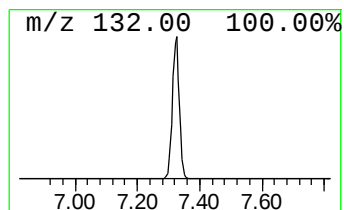
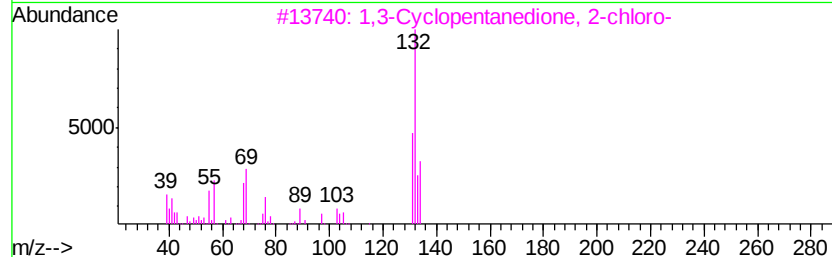
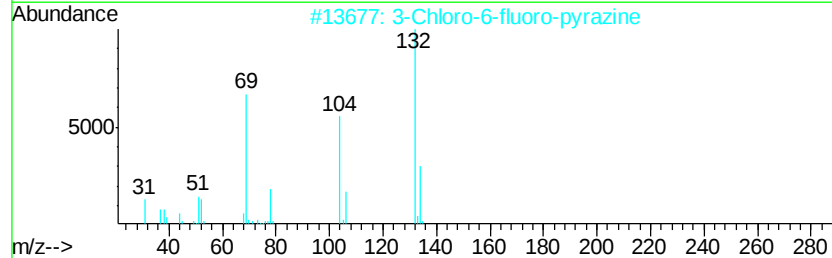
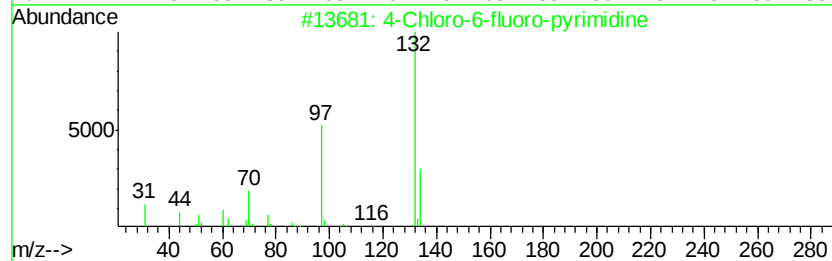
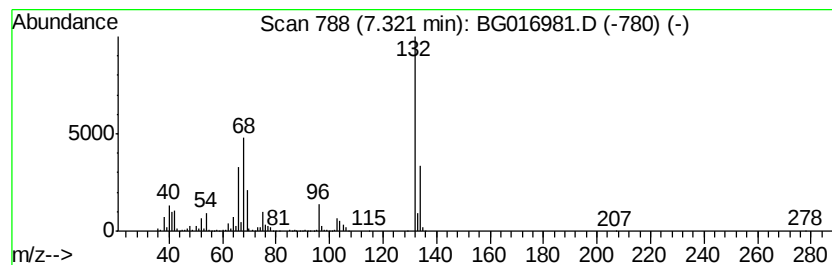
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	89.64 ng	1573800	1,4-Dichlorobenzene-d4	7.79

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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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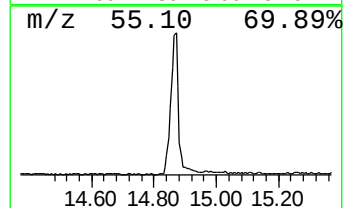
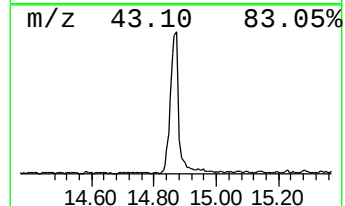
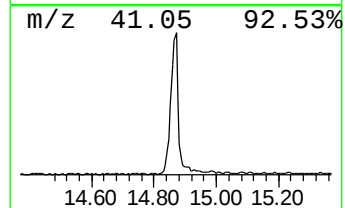
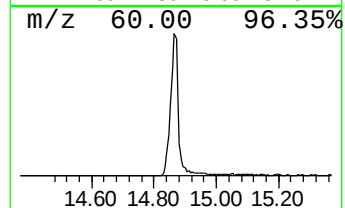
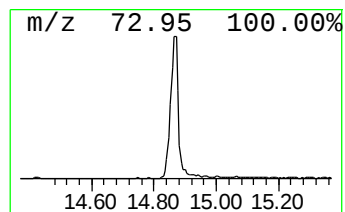
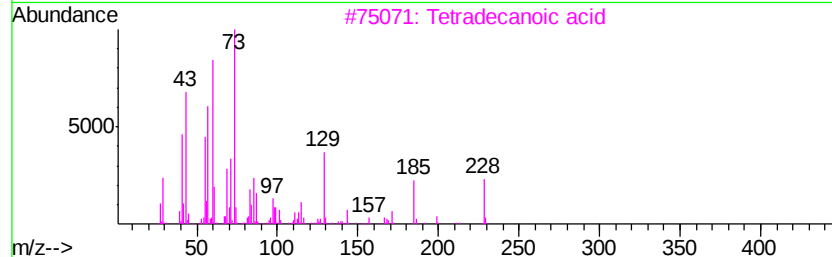
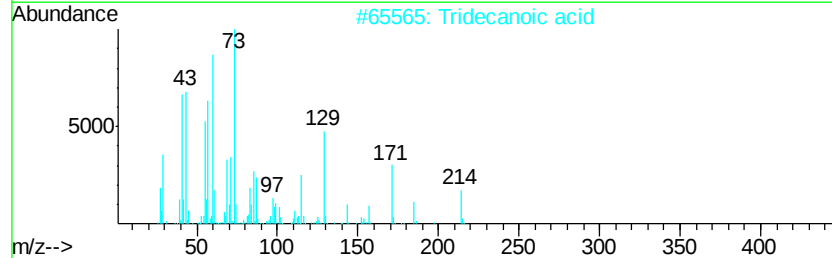
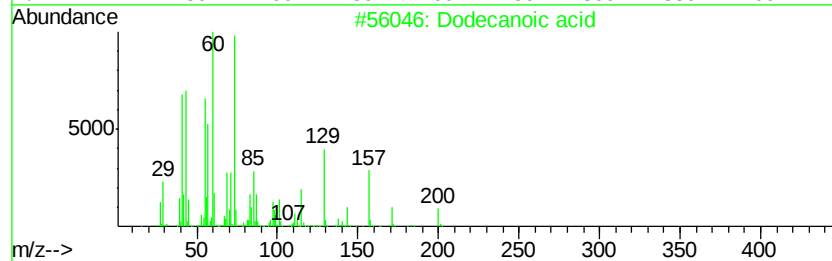
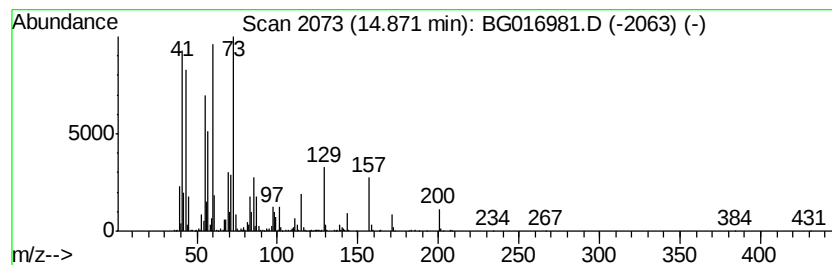
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Peak Number 6 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	33.61 ng	1361050	Acenaphthene-d10	14.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid	200 C12H24O2	000143-07-7	99
2	Tridecanoic acid	214 C13H26O2	000638-53-9	74
3	Tetradecanoic acid	228 C14H28O2	000544-63-8	64
4	Undecanoic acid	186 C11H22O2	000112-37-8	64
5	Nonanoic acid	158 C9H18O2	000112-05-0	46



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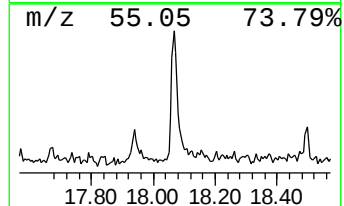
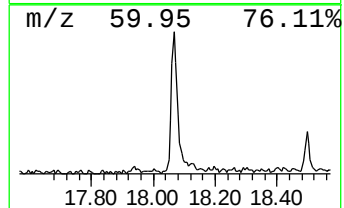
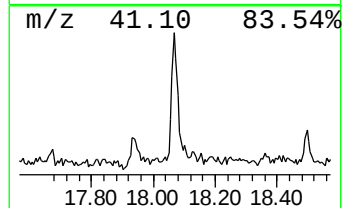
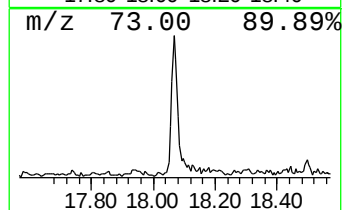
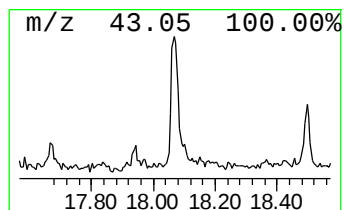
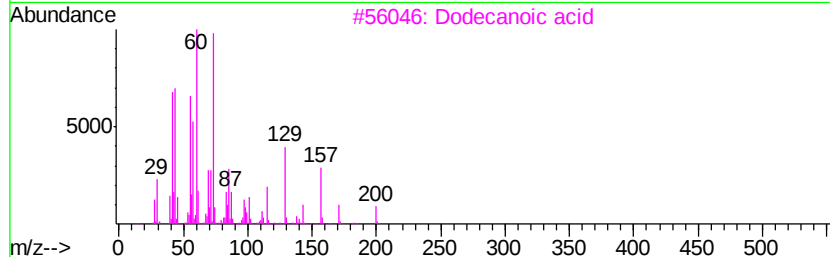
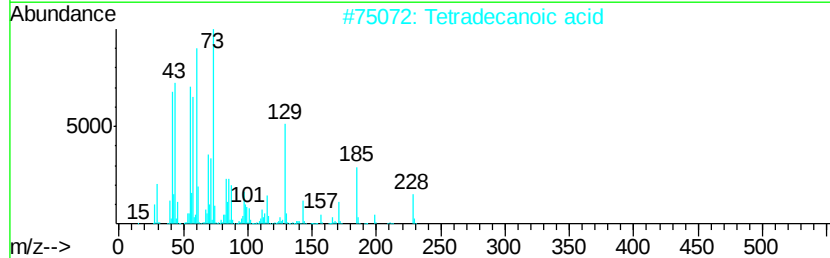
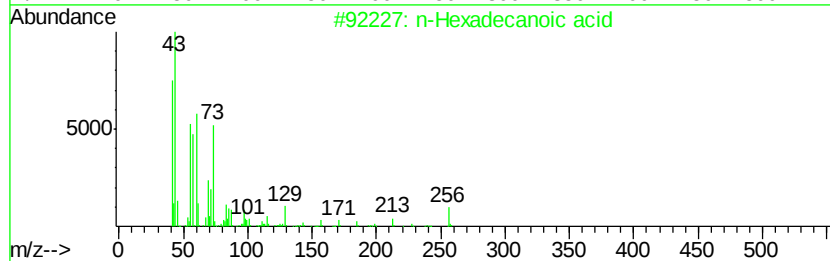
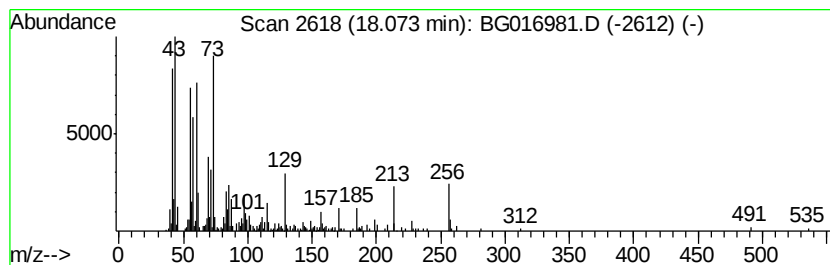
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	5.52 ng	290083	Phenanthrene-d10	17.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3		Dodecanoic acid	200	C12H24O2	000143-07-7	70
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Undecanoic acid	186	C11H22O2	000112-37-8	62



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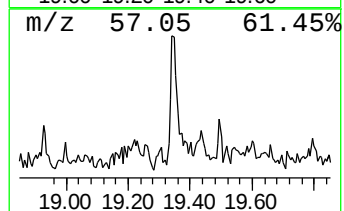
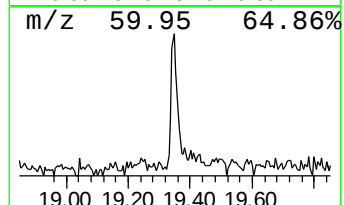
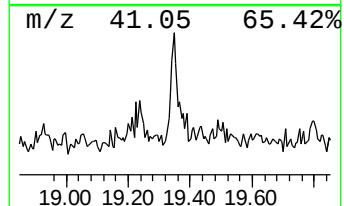
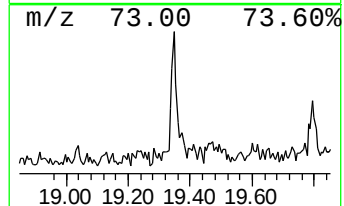
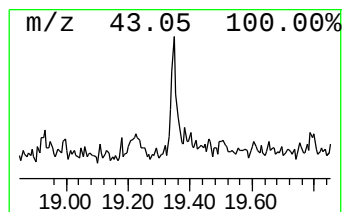
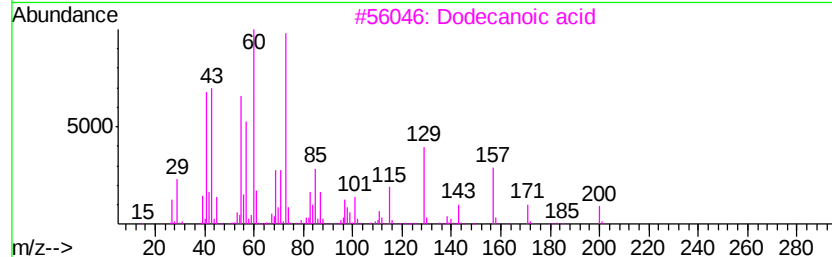
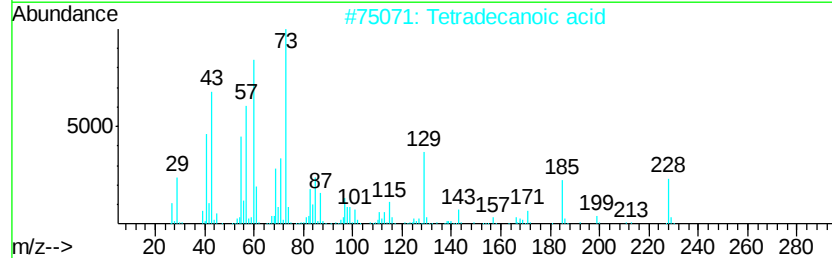
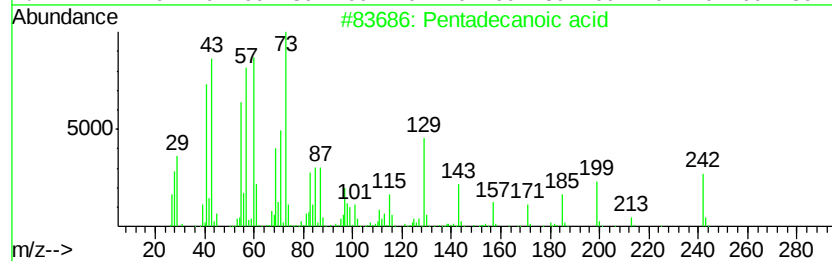
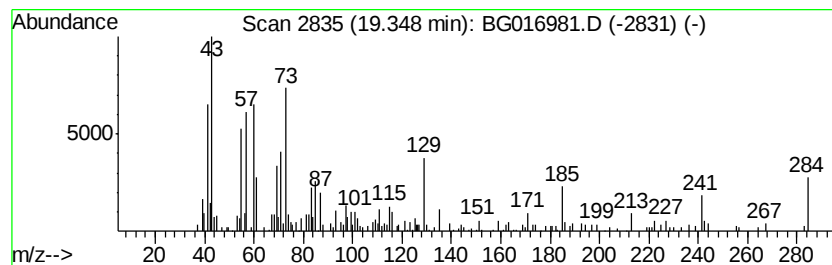
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BNA_G
ClientSampleId :
MPE-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.30 ng	137014	Chrysene-d12	21.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentadecanoic acid	242 C15H30O2	001002-84-2 93
2		Tetradecanoic acid	228 C14H28O2	000544-63-8 58
3		Dodecanoic acid	200 C12H24O2	000143-07-7 46
4		.beta.-D-Mannofuranoside, 1-O-(1...	332 C17H32O6	1000155-29-9 18
5		Heptanoic acid	130 C7H14O2	000111-14-8 18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-9

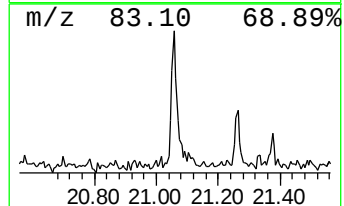
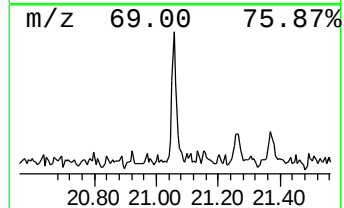
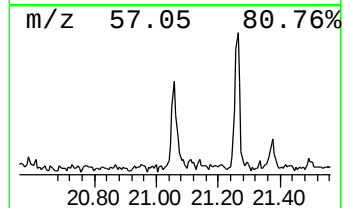
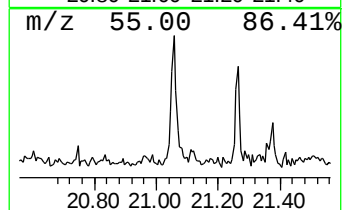
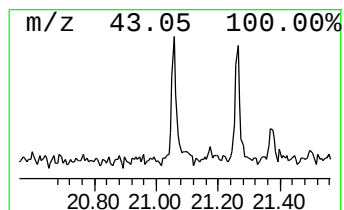
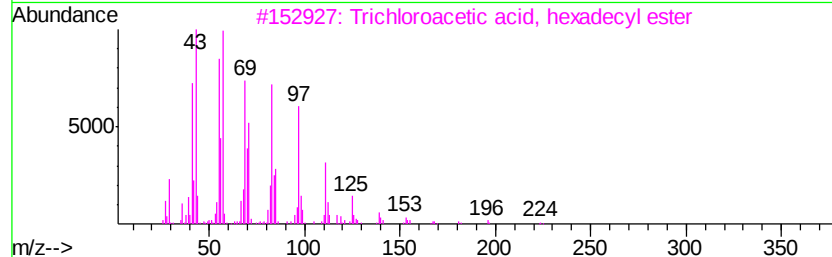
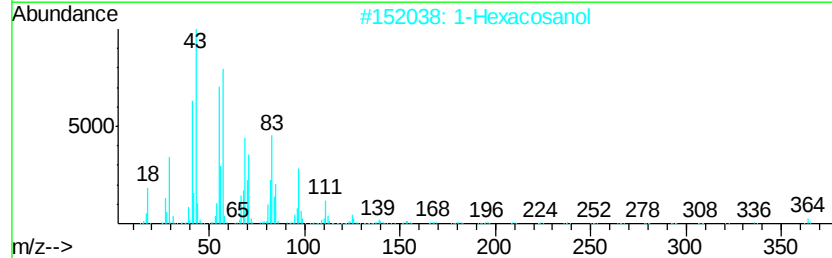
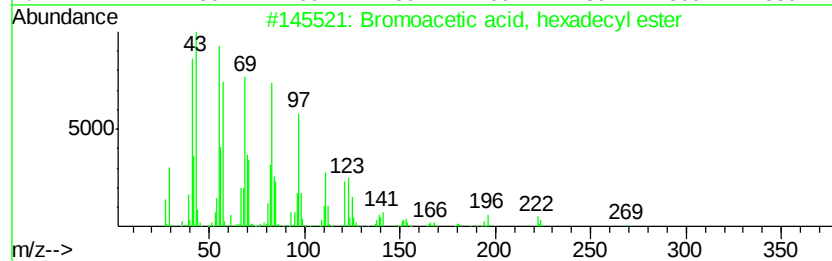
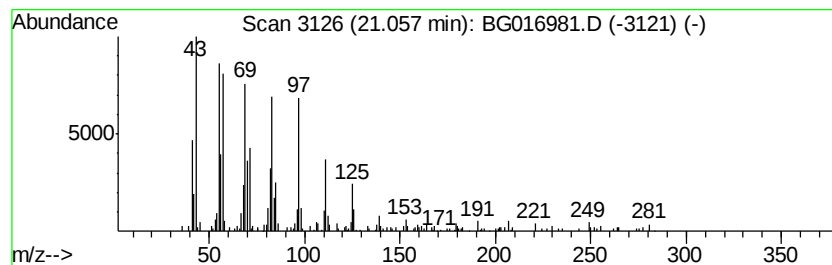
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	2.52 ng	150181	Chrysene-d12	21.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2		1-Hexacosanol	382	C26H54O	000506-52-5	74
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
4		1-Docosene	308	C22H44	001599-67-3	64
5		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-9

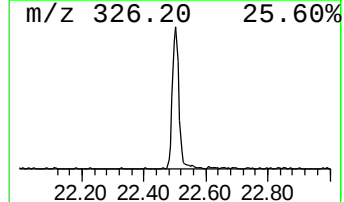
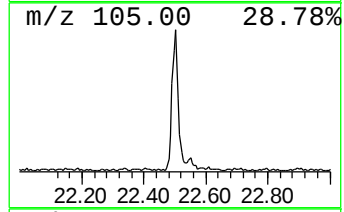
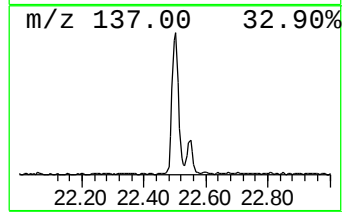
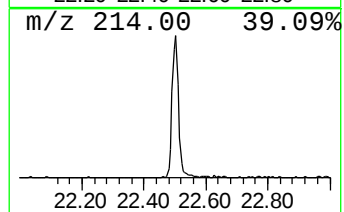
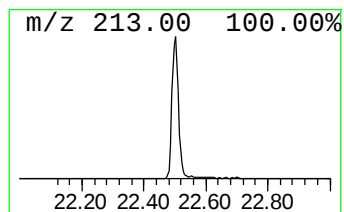
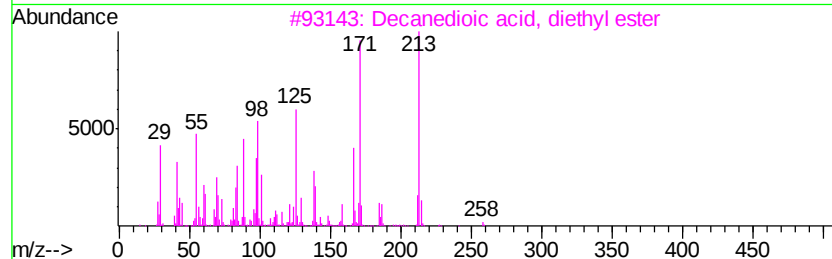
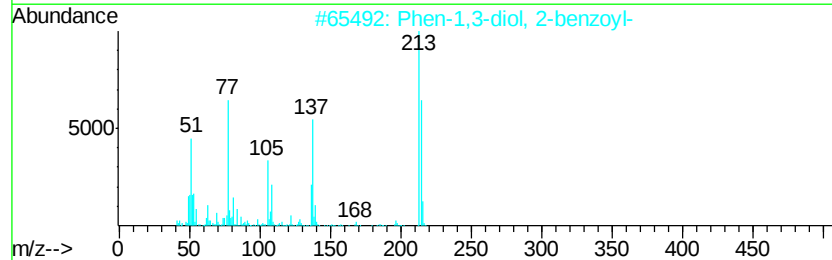
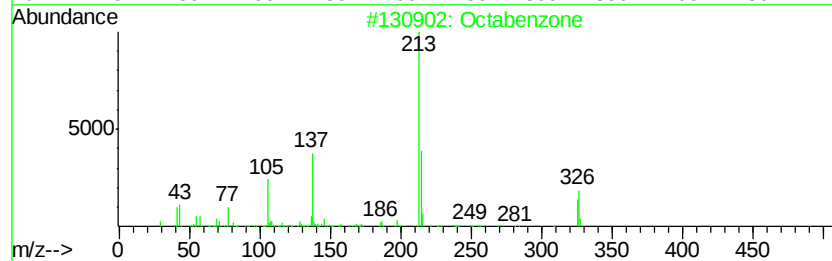
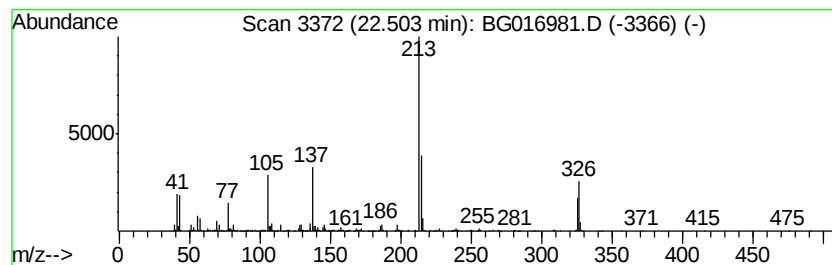
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octabenzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	15.70 ng	854923	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octabenzene	326	C21H26O3	001843-05-6	98
2		Phen-1,3-diol, 2-benzoyl-	214	C13H10O3	063411-81-4	32
3		Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	27
4		Naphthalene-2,6-dicarboxylic aci...	376	C24H24O4	1000189-60-8	17
5		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	17



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

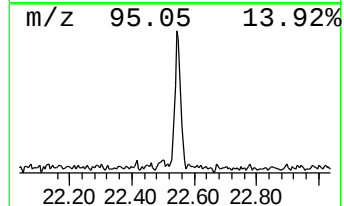
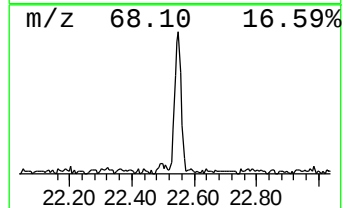
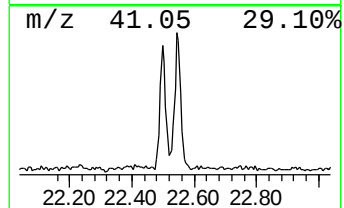
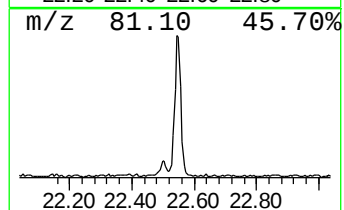
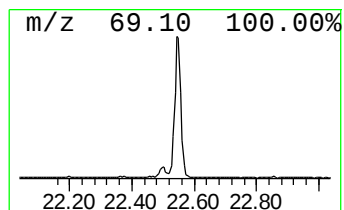
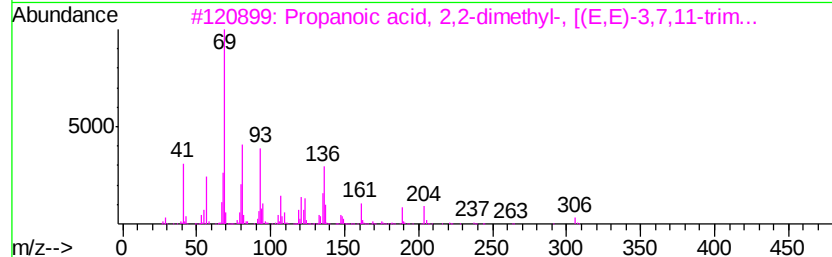
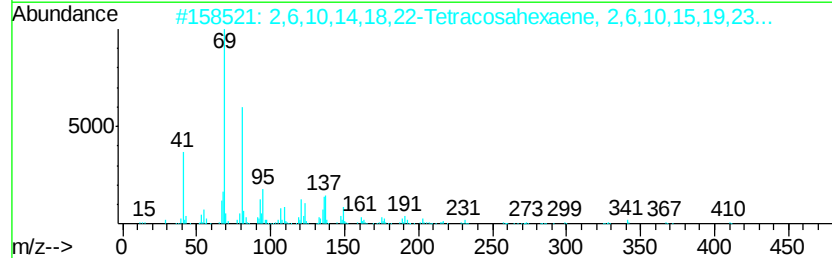
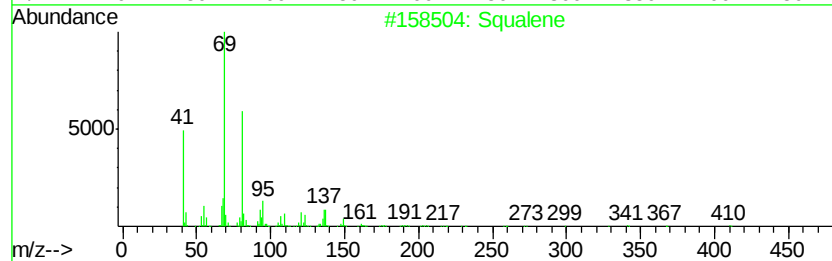
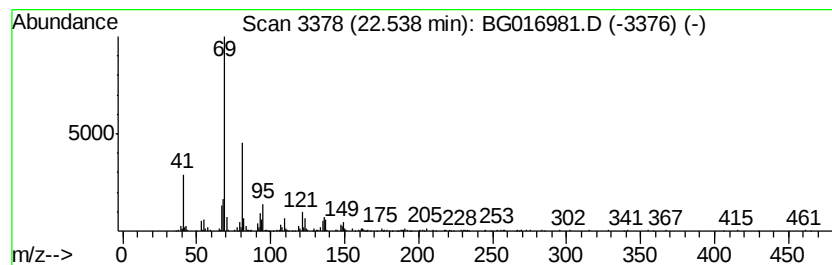
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	9.52 ng	518290	Perylene-d12	23.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 99
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 80
3	Propanoic acid, 2,2-dimethyl-, [...]		306 C20H34O2	1000164-38-8 72
4	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H24O	125529-10-4 72
5	Farnesol isomer a		222 C15H26O	1000108-92-4 72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
MPE-9

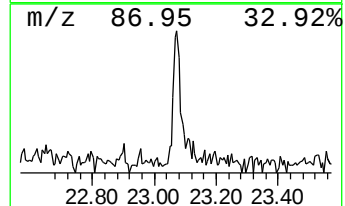
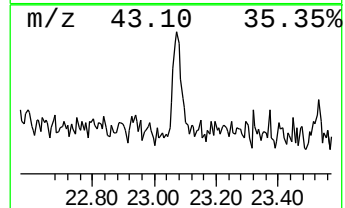
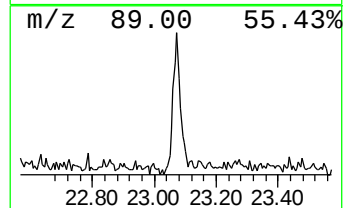
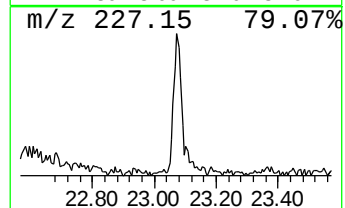
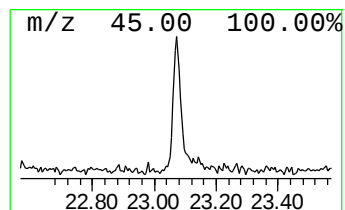
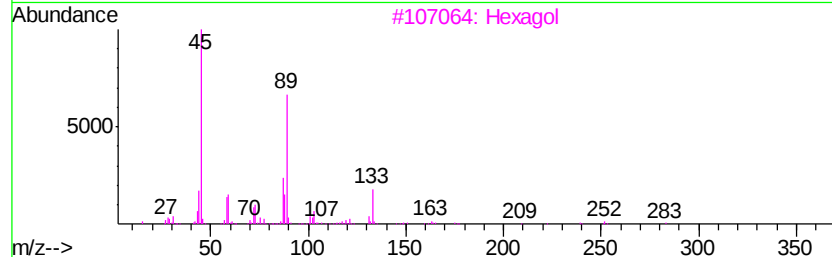
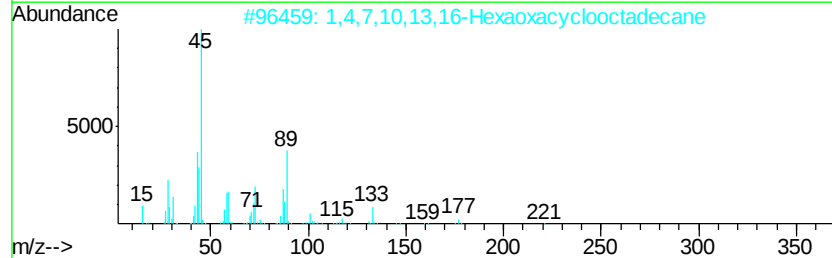
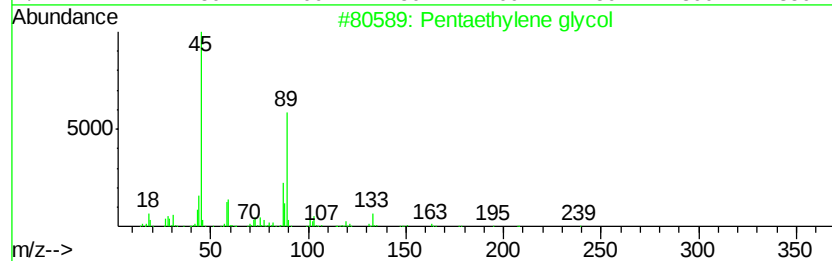
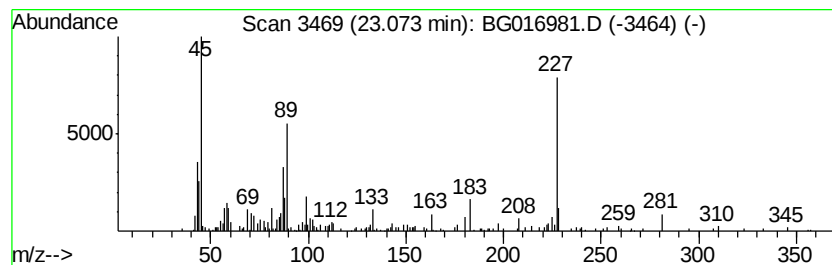
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown23.07 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.07	2.34 ng	127557	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentaethylene glycol	238	C10H22O6	004792-15-8	43
2		1,4,7,10,13,16-Hexaoxacyclooctadecane...	264	C12H24O6	017455-13-9	38
3		Hexagol	282	C12H26O7	002615-15-8	38
4		1,4,7,10,13,16-Hexaoxanonadecane...	318	C16H30O6	1000163-64-0	35
5		Octaethylene glycol	370	C16H34O9	1000289-34-2	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-9

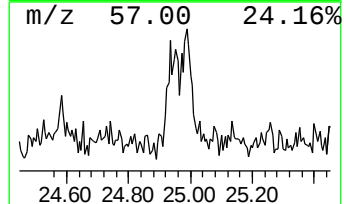
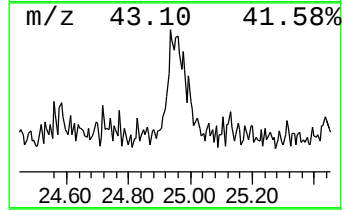
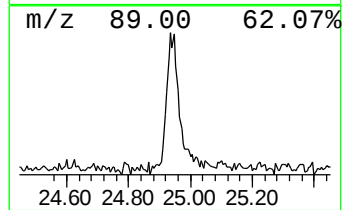
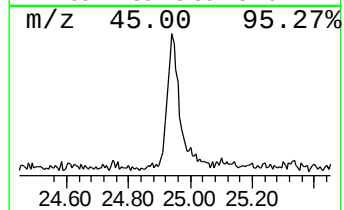
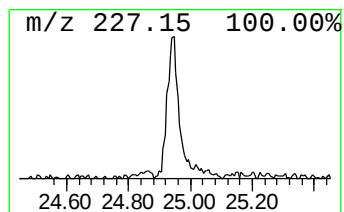
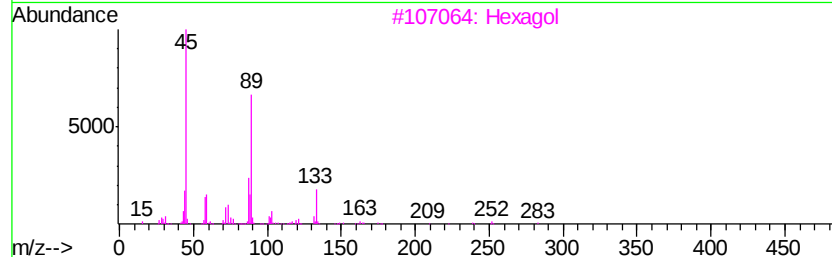
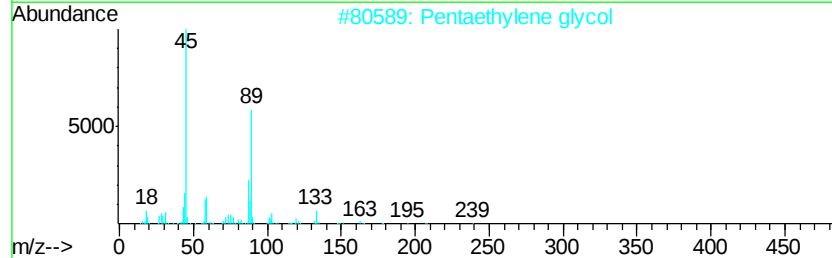
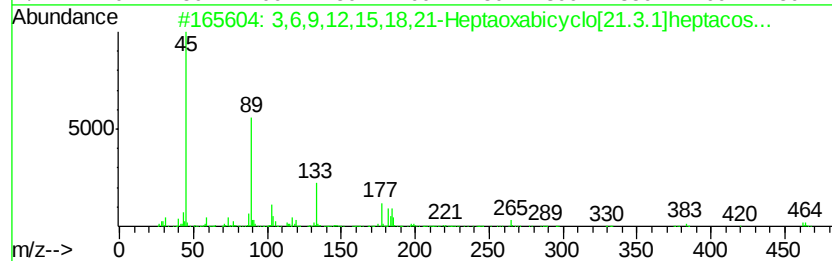
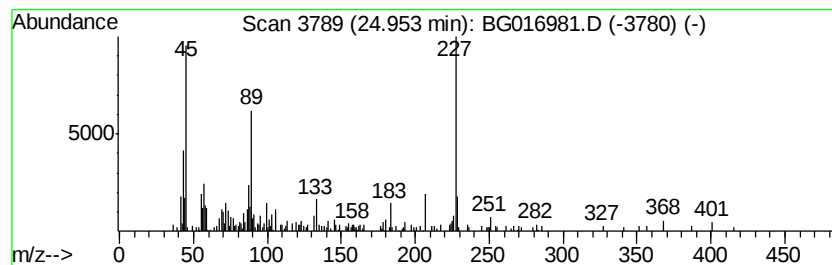
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown24.95 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.95	6.08 ng	331213	Perylene-d12	23.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15,18,21-Hepta	oxabicycl...	462	C20H31BrO7	111982-23-1	38	
2	Pentaethylene glycol		238	C10H22O6	004792-15-8	38	
3	Hexagol		282	C12H26O7	002615-15-8	38	
4	Benzoic acid, 3-(phenylamino)-, ...		227	C14H13NO2	055622-43-0	38	
5	2-Methyl-9-chloro-acridine		227	C14H10ClN	016492-09-4	38	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
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Misc :
ALS Vial : 29 Sample Multiplier: 1

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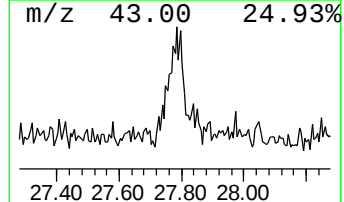
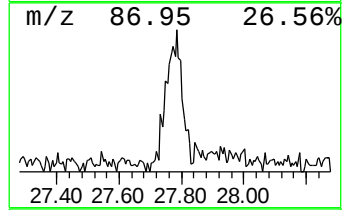
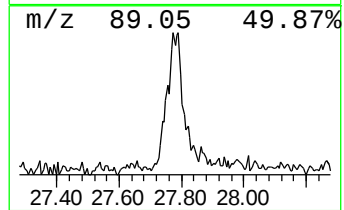
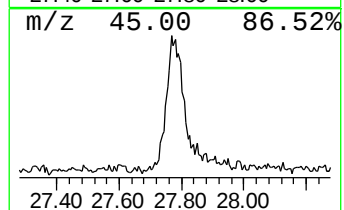
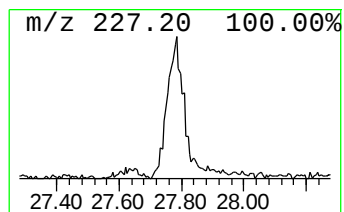
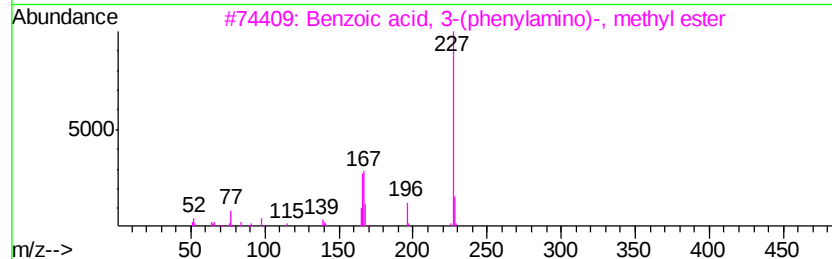
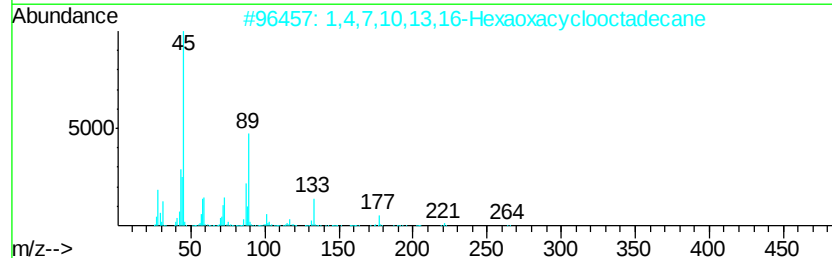
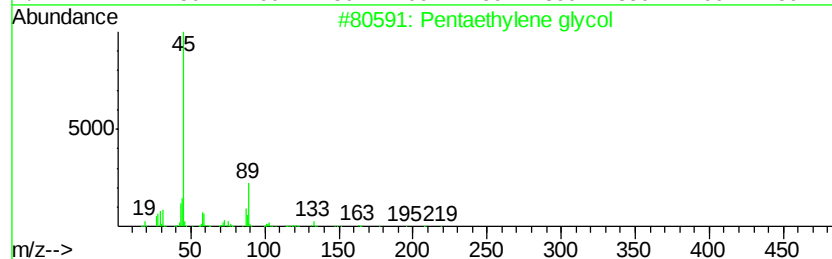
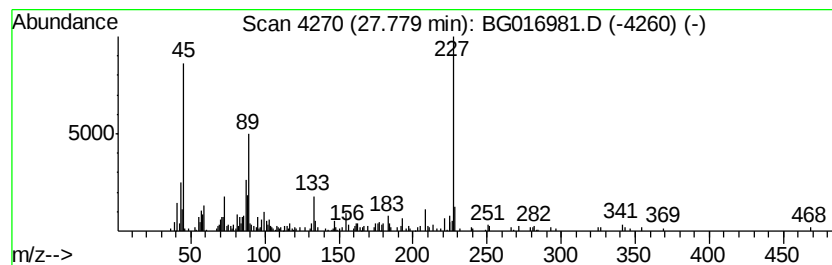
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown27.78 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.78	5.52 ng	300519	Perylene-d12	23.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentaethylene glycol	238	C10H22O6	004792-15-8	43
2			1,4,7,10,13,16-Hexaoxacyclooctadecane	264	C12H24O6	017455-13-9	43
3			Benzoic acid, 3-(phenylamino)-, ...	227	C14H13NO2	055622-43-0	38
4			2-(4'-Hydroxyphenyl)-2-(4'-methoxyphenyl)-	242	C16H18O2	016530-58-8	32
5			Heptane, 4-methoxy-3-(methoxymethyl)-	174	C10H22O2	020637-47-2	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016981.D
Acq On : 9 May 2015 7:39
Operator : TP/IZ
Sample : G2058-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.99	39.7	ng	697608	1	7.79	351123	20.0
unknown4.91	4.91	3.6	ng	62816	1	7.79	351123	20.0
unknown7.32	7.32	89.6	ng	1573800	1	7.79	351123	20.0
Dodecanoic acid	14.87	33.6	ng	1361050	3	14.43	809929	20.0
n-Hexadecanoic acid	18.07	5.5	ng	290083	4	17.17	1050410	20.0
Pentadecanoic acid	19.35	2.3	ng	137014	5	21.35	1193460	20.0
Bromoacetic acid,...	21.06	2.5	ng	150181	5	21.35	1193460	20.0
Octabenzene	22.50	15.7	ng	854923	6	23.64	1089150	20.0
Squalene	22.54	9.5	ng	518290	6	23.64	1089150	20.0
unknown23.07	23.07	2.3	ng	127557	6	23.64	1089150	20.0
unknown24.95	24.95	6.1	ng	331213	6	23.64	1089150	20.0
unknown27.78	27.78	5.5	ng	300519	6	23.64	1089150	20.0