

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016444.D
 Acq On : 16 Apr 2015 5:26
 Operator : TP/IZ
 Sample : G1829-14
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TE-PMW-40

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-BG040615.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	2.761	7	12	21	rBV	291233	465951	10.74%	1.774%
2	2.837	21	25	35	rVB	370019	454781	10.49%	1.731%
3	3.072	61	65	74	rVB	35358	50740	1.17%	0.193%
4	4.782	351	356	364	rVB2	54218	79680	1.84%	0.303%
5	5.258	430	437	453	rBV	682769	963503	22.22%	3.668%
6	6.180	590	594	602	rBV	27901	46354	1.07%	0.176%
7	6.856	700	709	722	rVB	465076	725374	16.73%	2.761%
8	7.203	761	768	781	rVB	1232140	1862058	42.94%	7.088%
9	7.667	840	847	854	rBV	293376	450536	10.39%	1.715%
10	7.984	894	901	910	rVB	929176	1434127	33.07%	5.459%
11	8.824	1036	1044	1053	rBV	854258	1336918	30.83%	5.089%
12	10.452	1313	1321	1328	rBV	445571	727367	16.77%	2.769%
13	12.655	1690	1696	1704	rBV	35380	60439	1.39%	0.230%
14	12.925	1735	1742	1749	rBV	2203356	3358242	77.44%	12.783%
15	14.306	1969	1977	1985	rBV2	692399	1056524	24.36%	4.022%
16	15.669	2203	2209	2215	rBV	70103	88761	2.05%	0.338%
17	15.798	2224	2231	2241	rBV	1677453	2402388	55.40%	9.145%
18	16.022	2265	2269	2271	rBV	32103	43530	1.00%	0.166%
19	16.075	2275	2278	2287	rVB	82354	116020	2.68%	0.442%
20	16.809	2400	2403	2408	rBV2	33735	44156	1.02%	0.168%
21	17.050	2437	2444	2454	rBV2	887472	1254571	28.93%	4.776%
22	17.549	2524	2529	2535	rBV	37674	47494	1.10%	0.181%
23	17.949	2592	2597	2606	rBV	244028	382913	8.83%	1.458%
24	18.043	2608	2613	2622	rVB	188609	268217	6.18%	1.021%
25	18.243	2643	2647	2651	rBV	37154	47605	1.10%	0.181%
26	18.877	2752	2755	2762	rBV	38870	43717	1.01%	0.166%
27	19.089	2787	2791	2793	rBV3	39528	59734	1.38%	0.227%
28	19.230	2811	2815	2832	rBV	179454	276283	6.37%	1.052%
29	19.494	2857	2860	2865	rVB	44674	49358	1.14%	0.188%
30	19.682	2886	2892	2897	rBV	3336864	4336584	100.00%	16.507%
31	20.481	3024	3028	3032	rBV3	71052	91677	2.11%	0.349%
32	20.910	3097	3101	3103	rBV	100879	113750	2.62%	0.433%
33	20.939	3103	3106	3116	rVB	361801	499680	11.52%	1.902%
34	21.145	3137	3141	3145	rBV	129192	143357	3.31%	0.546%

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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-BG040615.M
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35	21.227	3150	3155	3161	rVV	948637	1196287	27.59%	4.554%
36	21.380	3178	3181	3185	rVB	83696	89919	2.07%	0.342%
37	21.809	3250	3254	3265	rVB	79703	131630	3.04%	0.501%
38	22.067	3295	3298	3302	rVB2	40225	45851	1.06%	0.175%
39	22.267	3329	3332	3339	rVB2	76394	103924	2.40%	0.396%
40	22.391	3351	3353	3360	rVB	53708	67220	1.55%	0.256%
41	22.767	3414	3417	3422	rVB2	55707	76752	1.77%	0.292%
42	23.460	3528	3535	3550	rVB2	616967	1176499	27.13%	4.478%

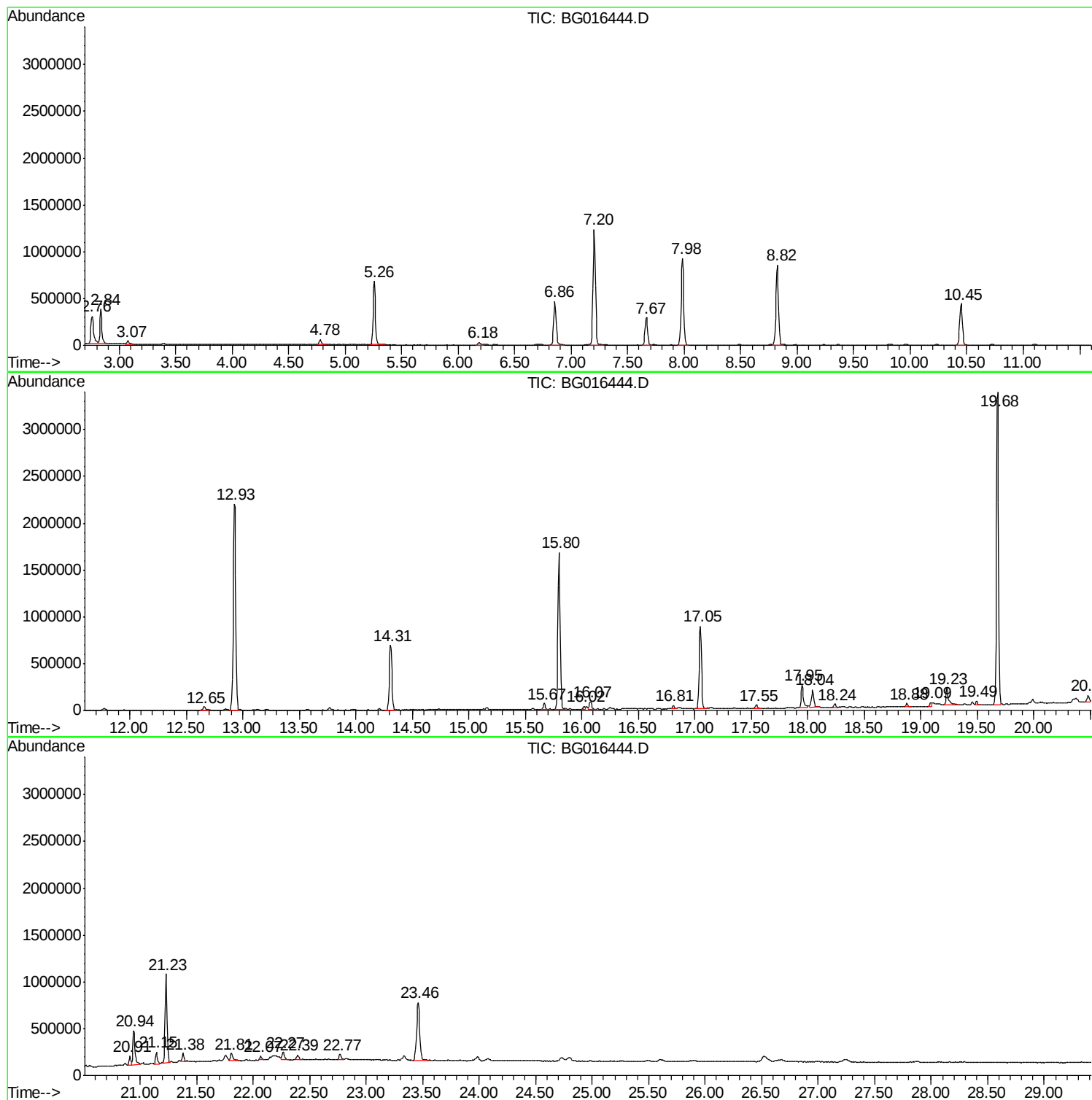
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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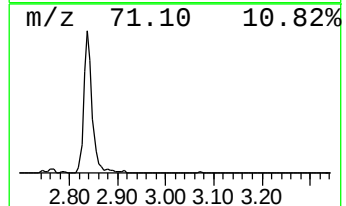
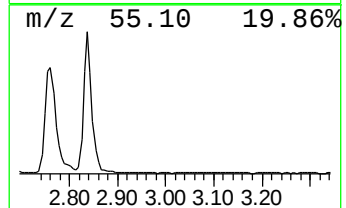
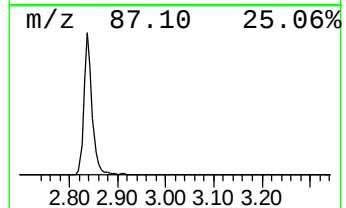
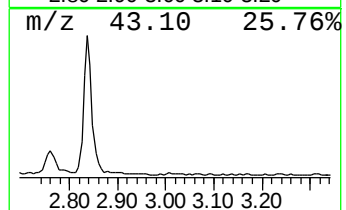
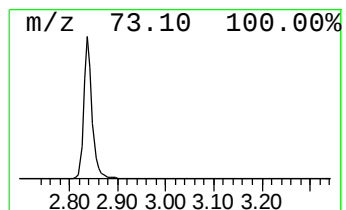
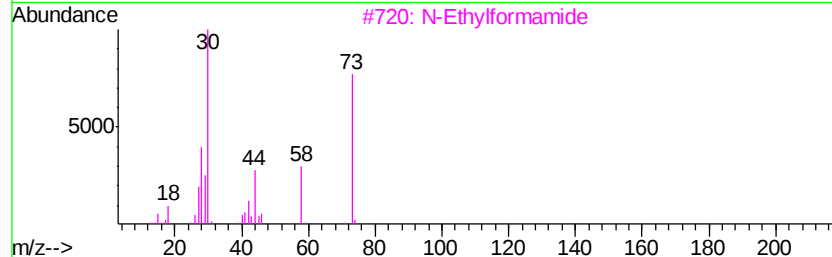
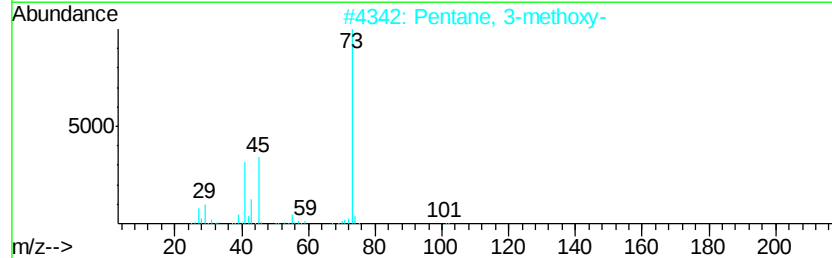
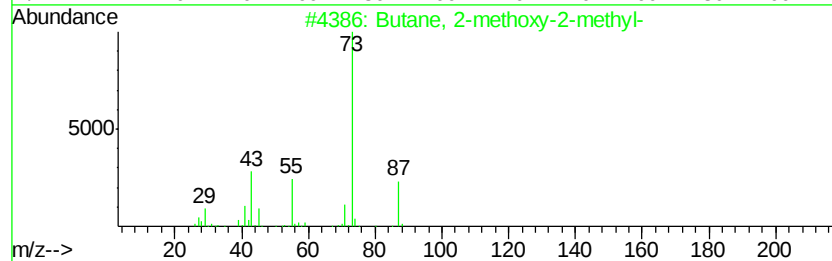
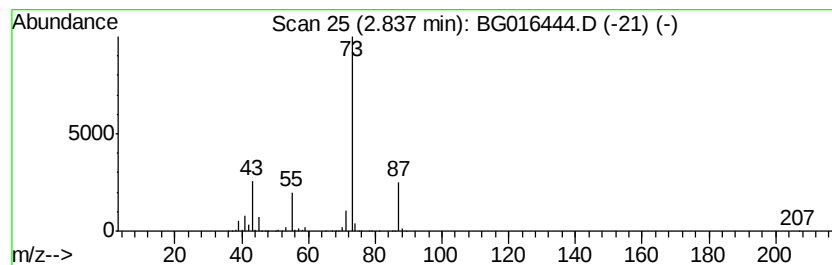
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	20.19 ng	454781	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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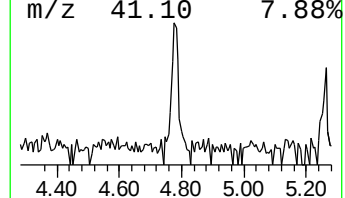
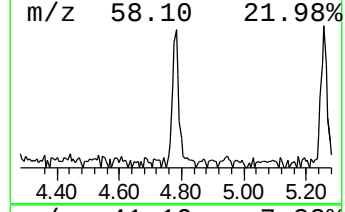
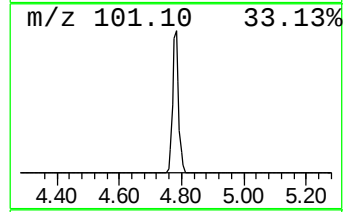
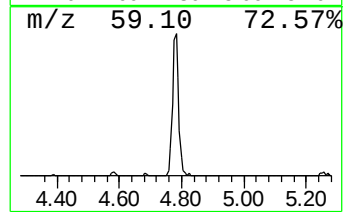
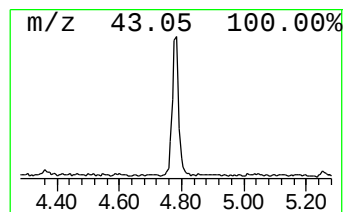
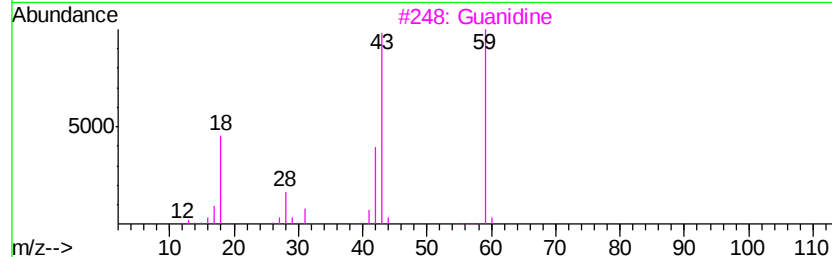
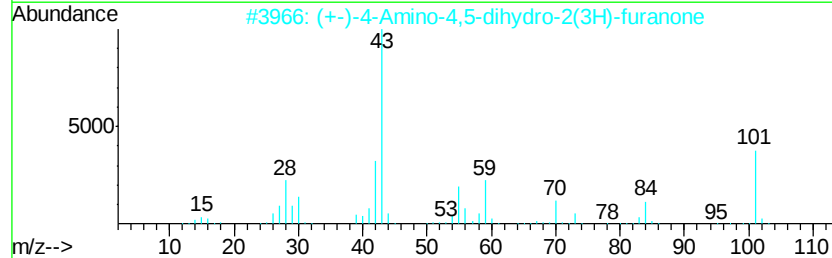
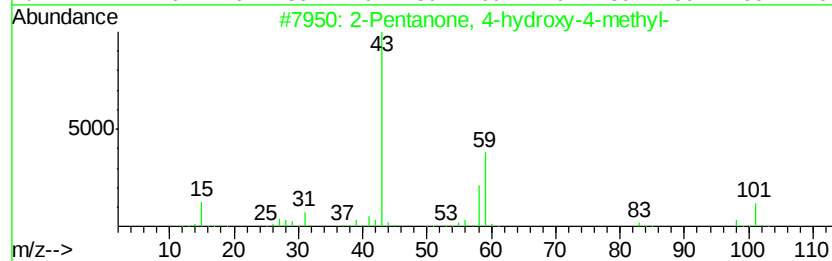
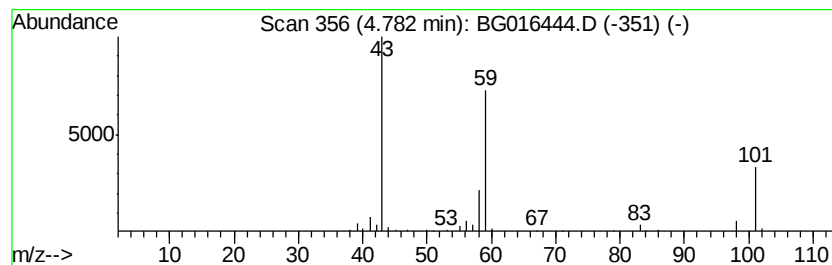
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.54 ng	79680	1,4-Dichlorobenzene-d4	7.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Guanidine	59	CH5N3	000113-00-8	38
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5			6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	17



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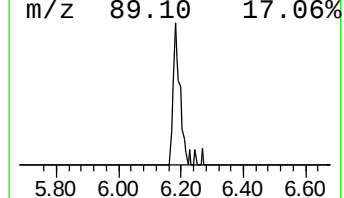
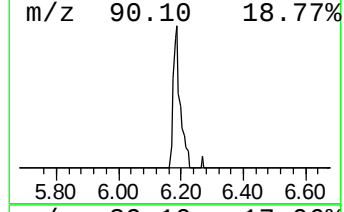
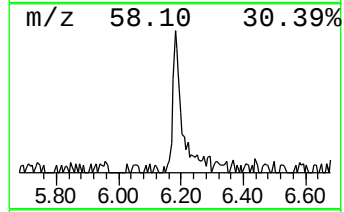
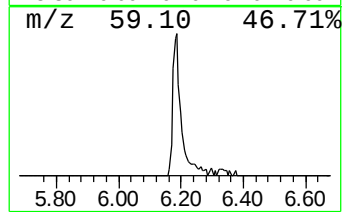
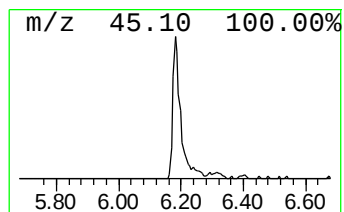
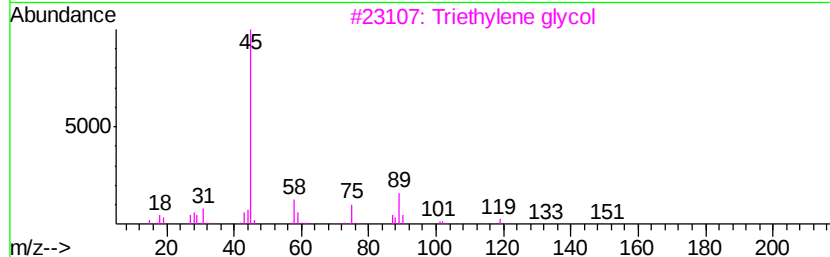
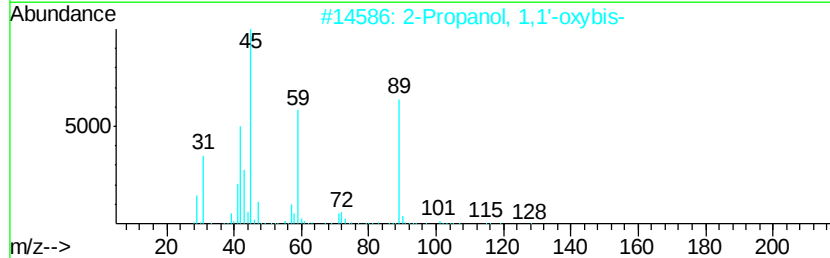
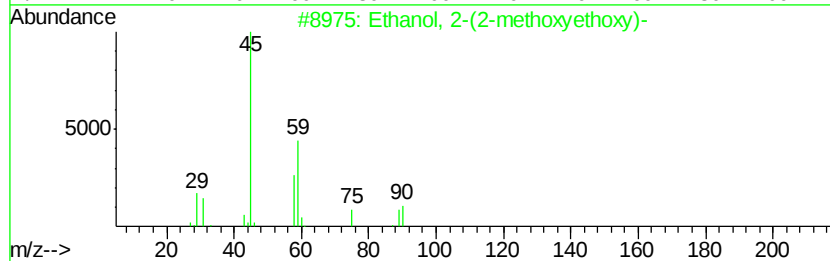
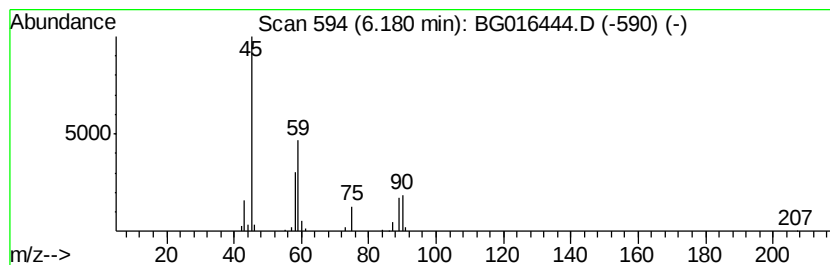
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	2.06 ng	46354	1,4-Dichlorobenzene-d4	7.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2		2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	36
3		Triethylene glycol	150	C6H14O4	000112-27-6	36
4		Paraldehyde	132	C6H12O3	000123-63-7	23
5		Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	9



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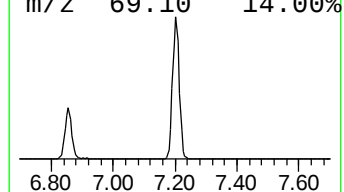
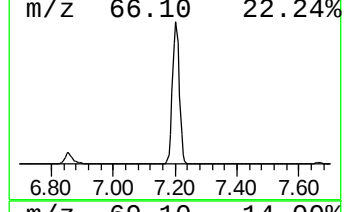
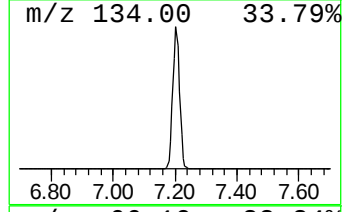
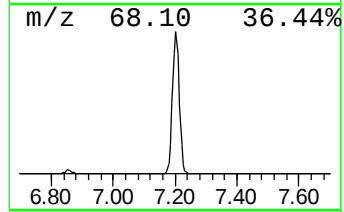
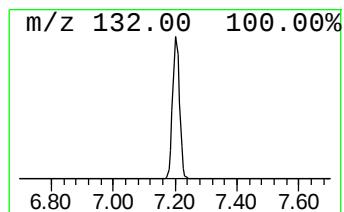
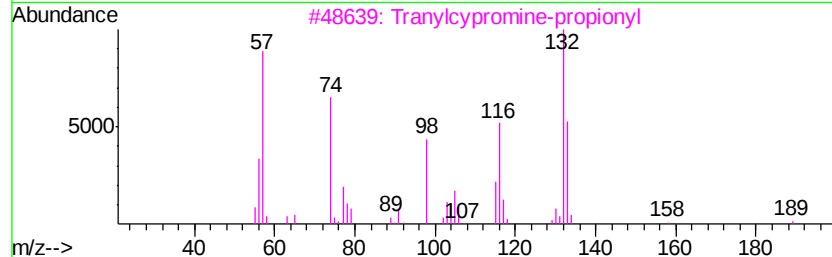
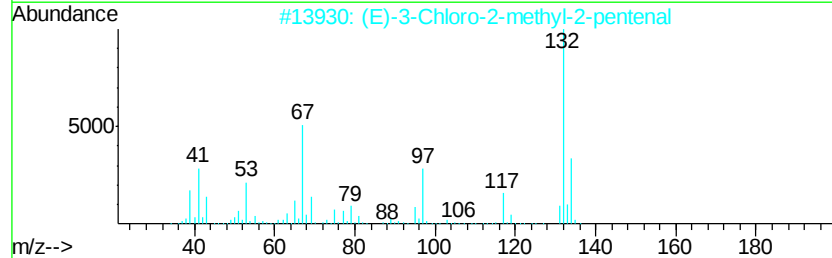
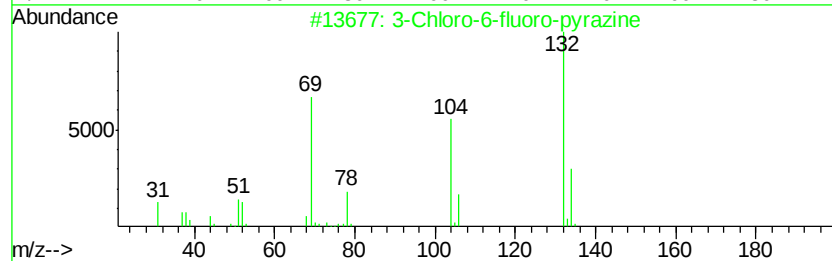
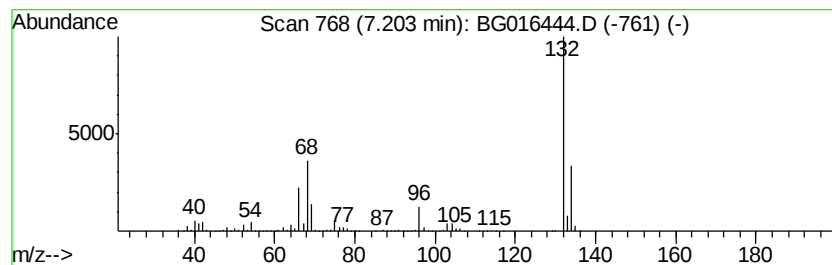
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	82.66 ng	1862060	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		Xenon	132	Xe	007440-63-3	9



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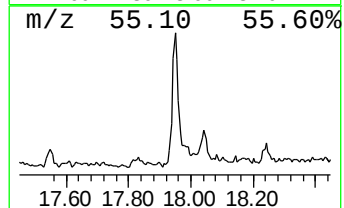
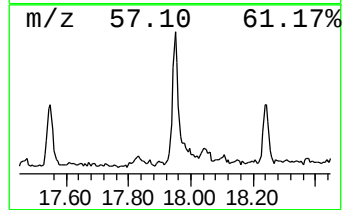
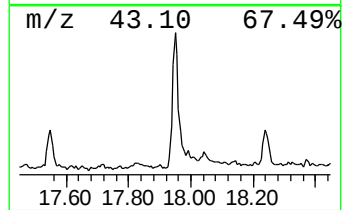
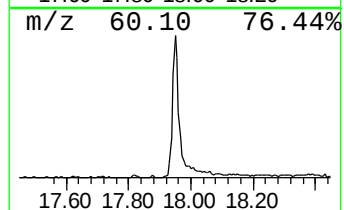
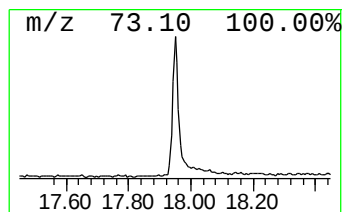
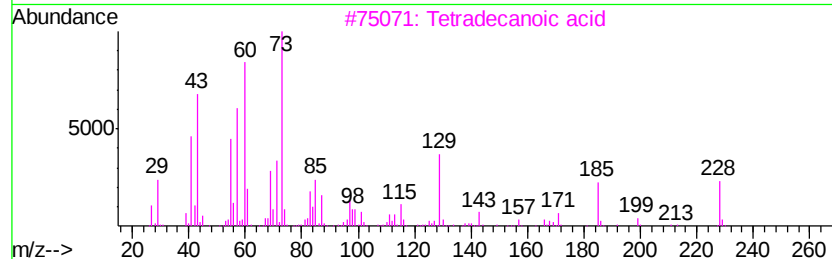
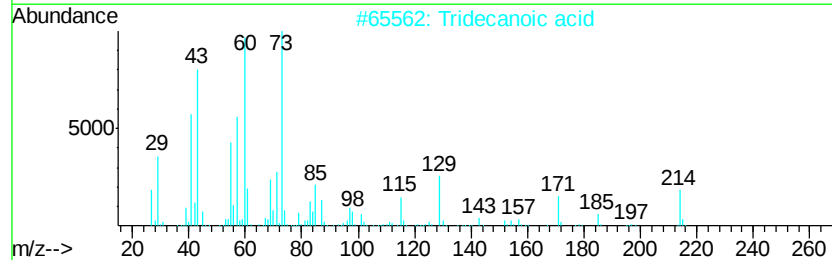
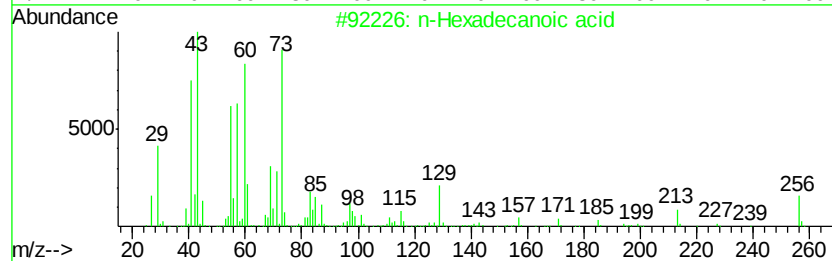
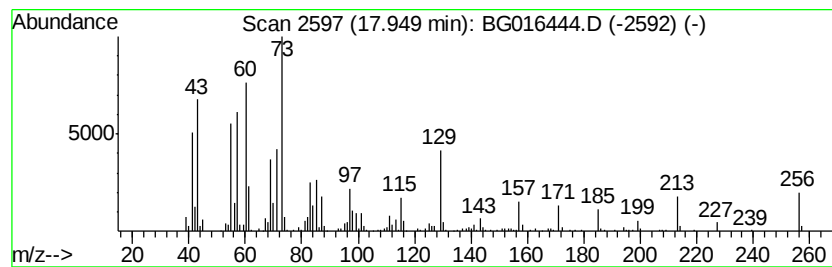
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TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.95	6.10 ng	382913	Phenanthrene-d10		17.05	
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	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016444.D
Acq On : 16 Apr 2015 5:26
Operator : TP/IZ
Sample : G1829-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

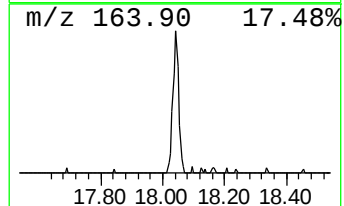
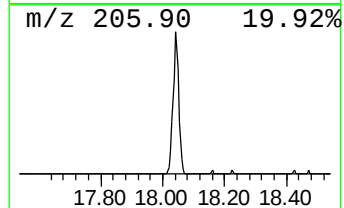
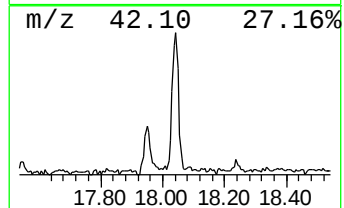
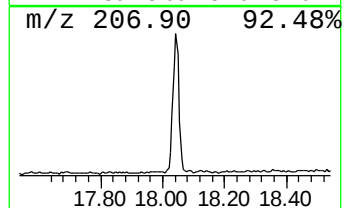
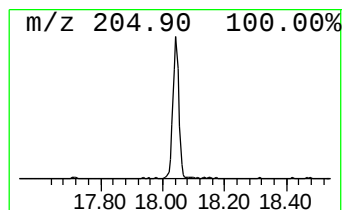
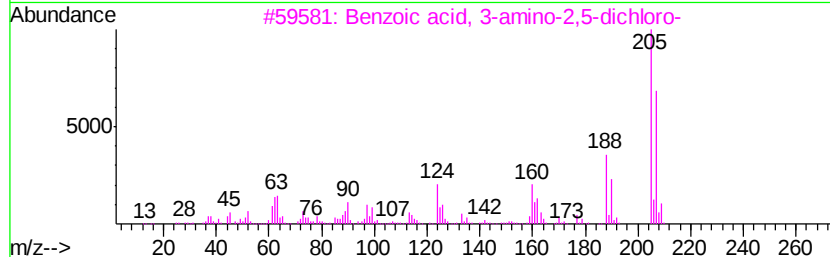
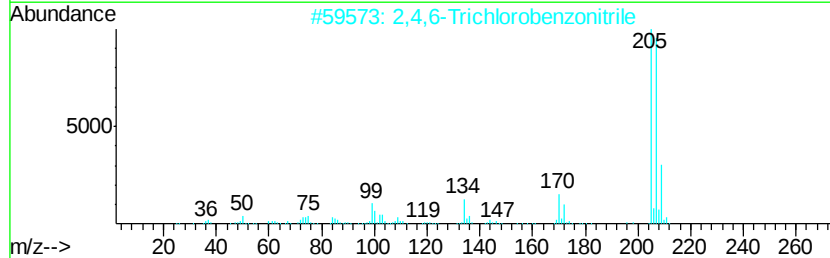
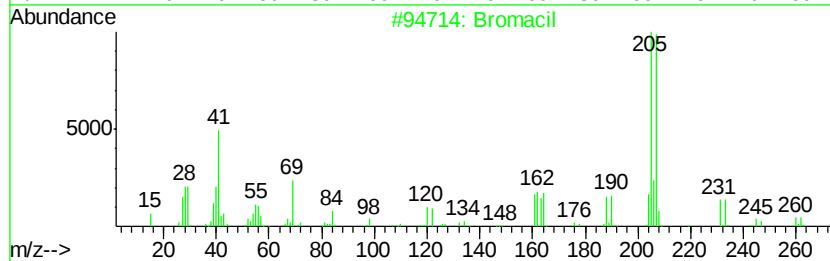
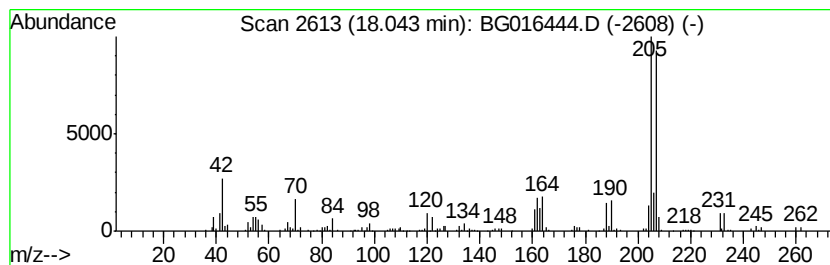
Instrument :
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ClientSampleId :
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromacil Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.04	4.28 ng	268217	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromacil	260	C9H13BrN2O2	000314-40-9	96
2	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	58
3	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	45
4	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	43
5	5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016444.D
Acq On : 16 Apr 2015 5:26
Operator : TP/IZ
Sample : G1829-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

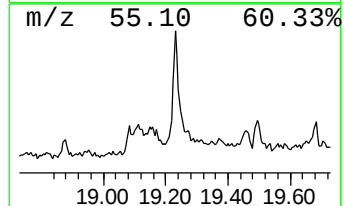
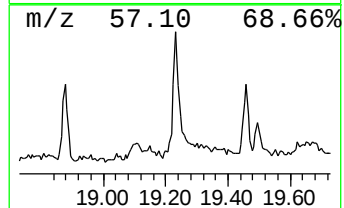
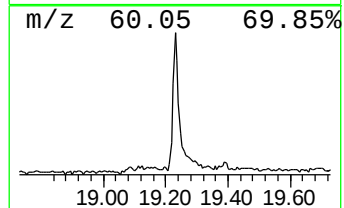
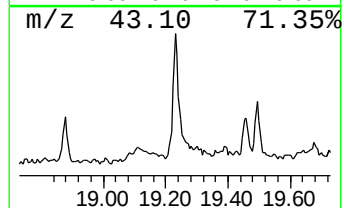
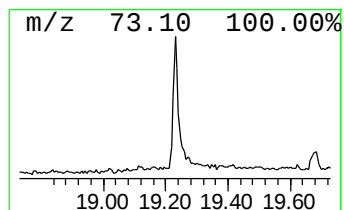
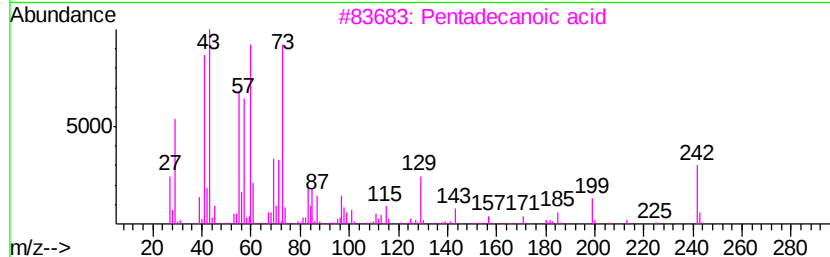
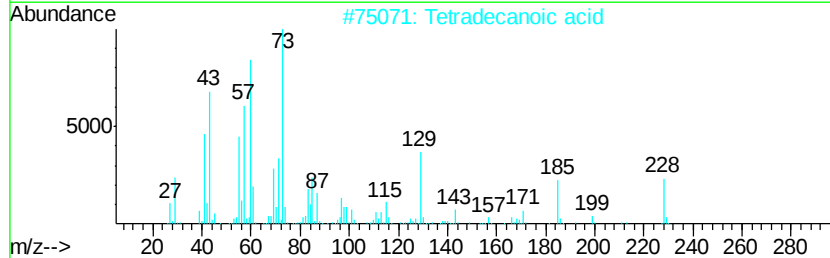
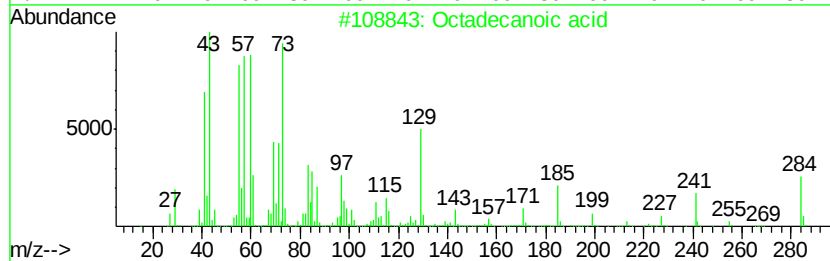
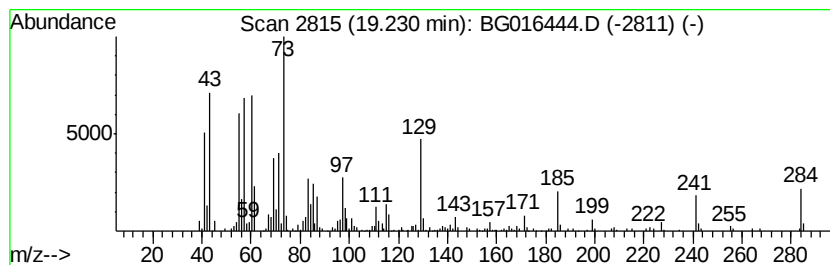
Instrument :
BNA_G
ClientSampleId :
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.23	4.62 ng	276283	Chrysene-d12	21.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
5	Undecanoic acid	186	C11H22O2	000112-37-8	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016444.D
Acq On : 16 Apr 2015 5:26
Operator : TP/IZ
Sample : G1829-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

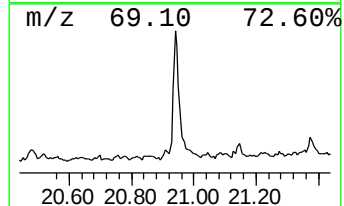
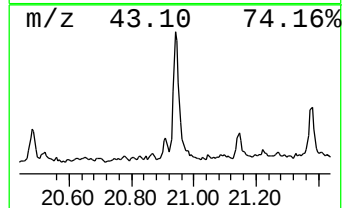
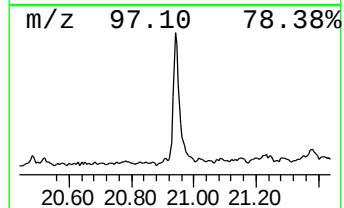
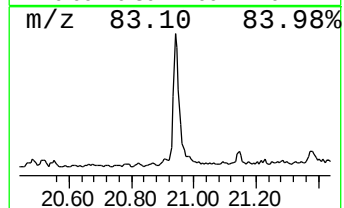
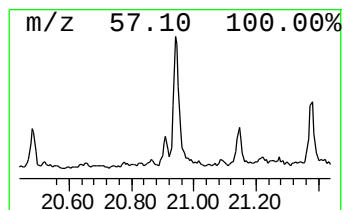
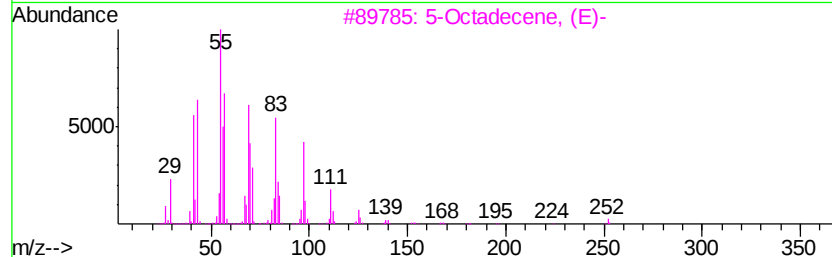
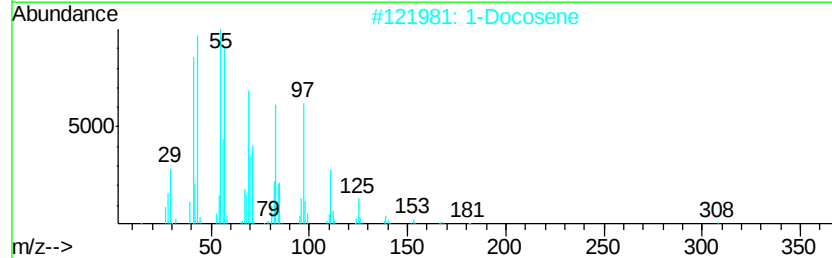
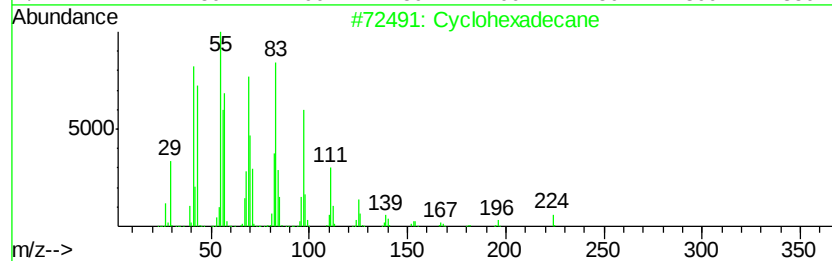
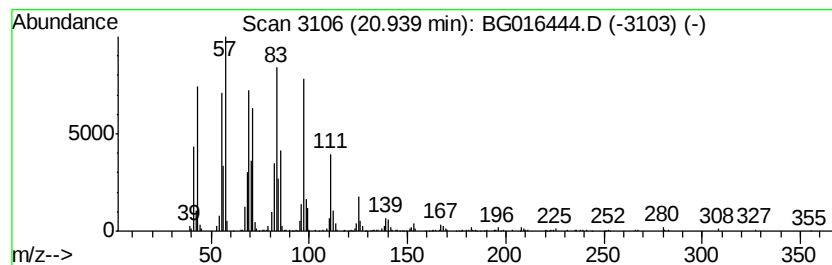
Instrument :
BNA_G
ClientSampleId :
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.94	8.35 ng	499680	Chrysene-d12	21.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Docosene	308	C22H44	001599-67-3	95
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016444.D
Acq On : 16 Apr 2015 5:26
Operator : TP/IZ
Sample : G1829-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

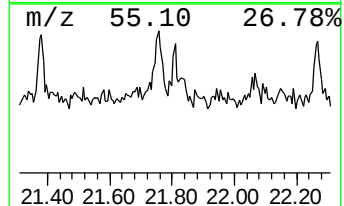
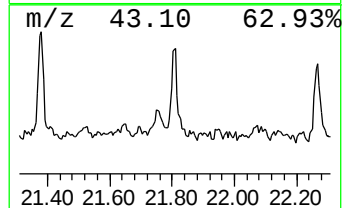
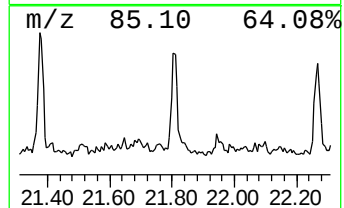
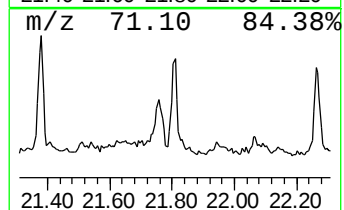
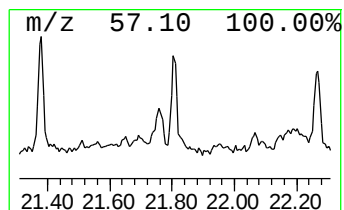
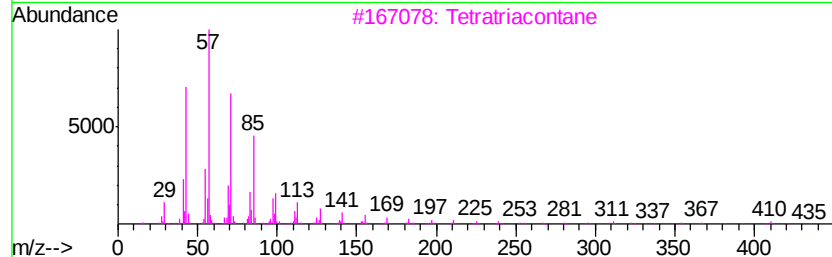
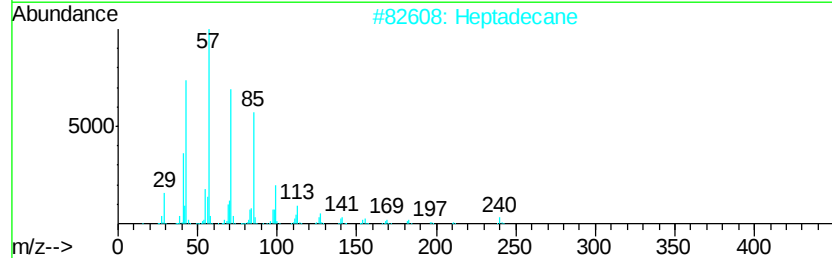
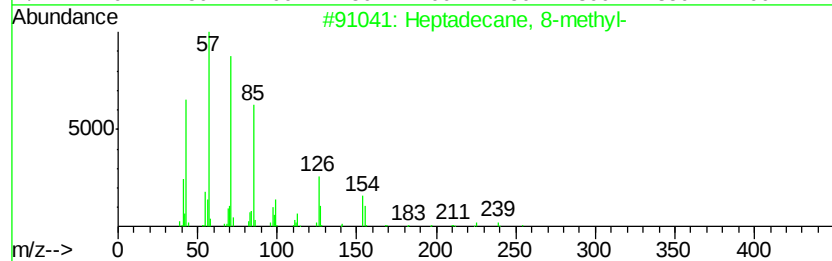
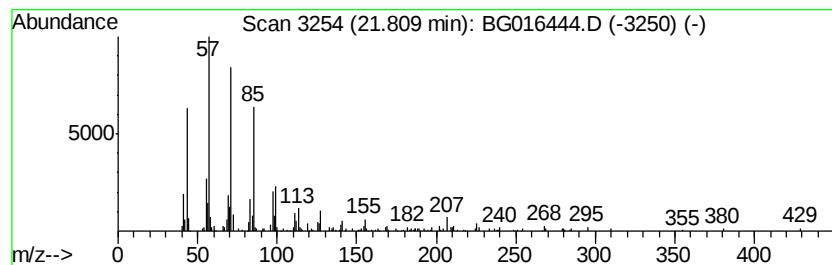
Instrument :
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ClientSampleId :
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 8-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.20 ng	131630	Chrysene-d12	21.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heptadecane, 8-methyl-	254 C18H38	013287-23-5 91
2		Heptadecane	240 C17H36	000629-78-7 91
3		Tetratriacontane	479 C34H70	014167-59-0 87
4		Nonadecane, 9-methyl-	282 C20H42	013287-24-6 86
5		Dodecane, 2-methyl-	184 C13H28	001560-97-0 81



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016444.D
Acq On : 16 Apr 2015 5:26
Operator : TP/IZ
Sample : G1829-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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...	2.84	20.2	ng	454781	1	7.67	450536	20.0
2-Pentanone, 4-hy...	4.78	3.5	ng	79680	1	7.67	450536	20.0
Ethanol, 2-(2-met...	6.18	2.1	ng	46354	1	7.67	450536	20.0
unknown7.20	7.20	82.7	ng	1862060	1	7.67	450536	20.0
n-Hexadecanoic acid	17.95	6.1	ng	382913	4	17.05	1254570	20.0
Bromacil	18.04	4.3	ng	268217	4	17.05	1254570	20.0
Octadecanoic acid	19.23	4.6	ng	276283	5	21.23	1196290	20.0
Cyclohexadecane	20.94	8.3	ng	499680	5	21.23	1196290	20.0
Heptadecane, 8-me...	21.81	2.2	ng	131630	5	21.23	1196290	20.0