

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
 Data File : BG019965.D
 Acq On : 6 Dec 2015 13:50
 Operator : UM/NP
 Sample : G4650-15
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COFF(0-2)-3

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-BG120215.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	2.991	22	26	34	rBV	41882	62506	3.29%	0.509%
2	5.189	393	400	409	rBV	100293	152189	8.02%	1.238%
3	5.659	473	480	489	rVB	436287	690163	36.37%	5.615%
4	7.257	744	752	765	rVB	493393	867758	45.73%	7.060%
5	7.639	809	817	826	rBV	467943	807072	42.53%	6.566%
6	8.115	892	898	904	rBV	117886	194517	10.25%	1.583%
7	8.438	946	953	961	rBV	316220	537410	28.32%	4.372%
8	9.278	1087	1096	1106	rBV	317782	561167	29.57%	4.566%
9	10.929	1369	1377	1387	rVB	165868	295926	15.59%	2.408%
10	13.367	1783	1792	1801	rBV	843898	1268434	66.84%	10.320%
11	14.184	1925	1931	1940	rBV	173660	258132	13.60%	2.100%
12	14.625	2001	2006	2015	rBV	24103	34532	1.82%	0.281%
13	14.742	2019	2026	2033	rVB2	287116	457531	24.11%	3.723%
14	15.541	2154	2162	2164	rBV2	13583	22460	1.18%	0.183%
15	15.576	2164	2168	2173	rVB	40400	53566	2.82%	0.436%
16	15.982	2226	2237	2242	rBV3	12918	31768	1.67%	0.258%
17	16.223	2268	2278	2286	rBV	721885	1082288	57.03%	8.806%
18	16.434	2309	2314	2317	rBV	41502	58116	3.06%	0.473%
19	17.063	2416	2421	2429	rBV	21655	34842	1.84%	0.283%
20	17.227	2443	2449	2453	rBV	24427	33325	1.76%	0.271%
21	17.480	2483	2492	2499	rBV2	375764	596738	31.44%	4.855%
22	18.356	2633	2641	2648	rBV	54206	81576	4.30%	0.664%
23	18.878	2724	2730	2734	rBV2	16432	28526	1.50%	0.232%
24	19.131	2769	2773	2781	rVB2	12727	22374	1.18%	0.182%
25	19.213	2782	2787	2791	rVV	34642	45749	2.41%	0.372%
26	19.278	2795	2798	2806	rVB	14273	20212	1.07%	0.164%
27	19.625	2852	2857	2860	rBV5	25793	35806	1.89%	0.291%
28	19.772	2876	2882	2887	rBV3	68924	114559	6.04%	0.932%
29	19.889	2898	2902	2905	rVB2	20557	24445	1.29%	0.199%
30	20.083	2929	2935	2940	rBV	1435259	1897766	100.00%	15.440%
31	20.289	2965	2970	2974	rBV	22657	31950	1.68%	0.260%
32	20.764	3044	3051	3056	rBV	27845	44857	2.36%	0.365%
33	20.811	3056	3059	3062	rBV	51840	60944	3.21%	0.496%
34	20.982	3084	3088	3090	rBV	17741	20640	1.09%	0.168%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.029	3093	3096	3100	rVB2	26748	30879	1.63%	0.251%
36	21.387	3153	3157	3166	rVB2	80517	127551	6.72%	1.038%
37	21.540	3180	3183	3187	rVB2	22595	30104	1.59%	0.245%
38	21.757	3213	3220	3227	rBV	455883	769321	40.54%	6.259%
39	21.951	3249	3253	3257	rVB2	19110	28181	1.48%	0.229%
40	22.092	3273	3277	3284	rVB2	15245	24955	1.31%	0.203%
41	23.273	3475	3478	3488	rVB8	12659	23623	1.24%	0.192%
42	25.036	3767	3778	3794	rVB	252482	726433	38.28%	5.910%

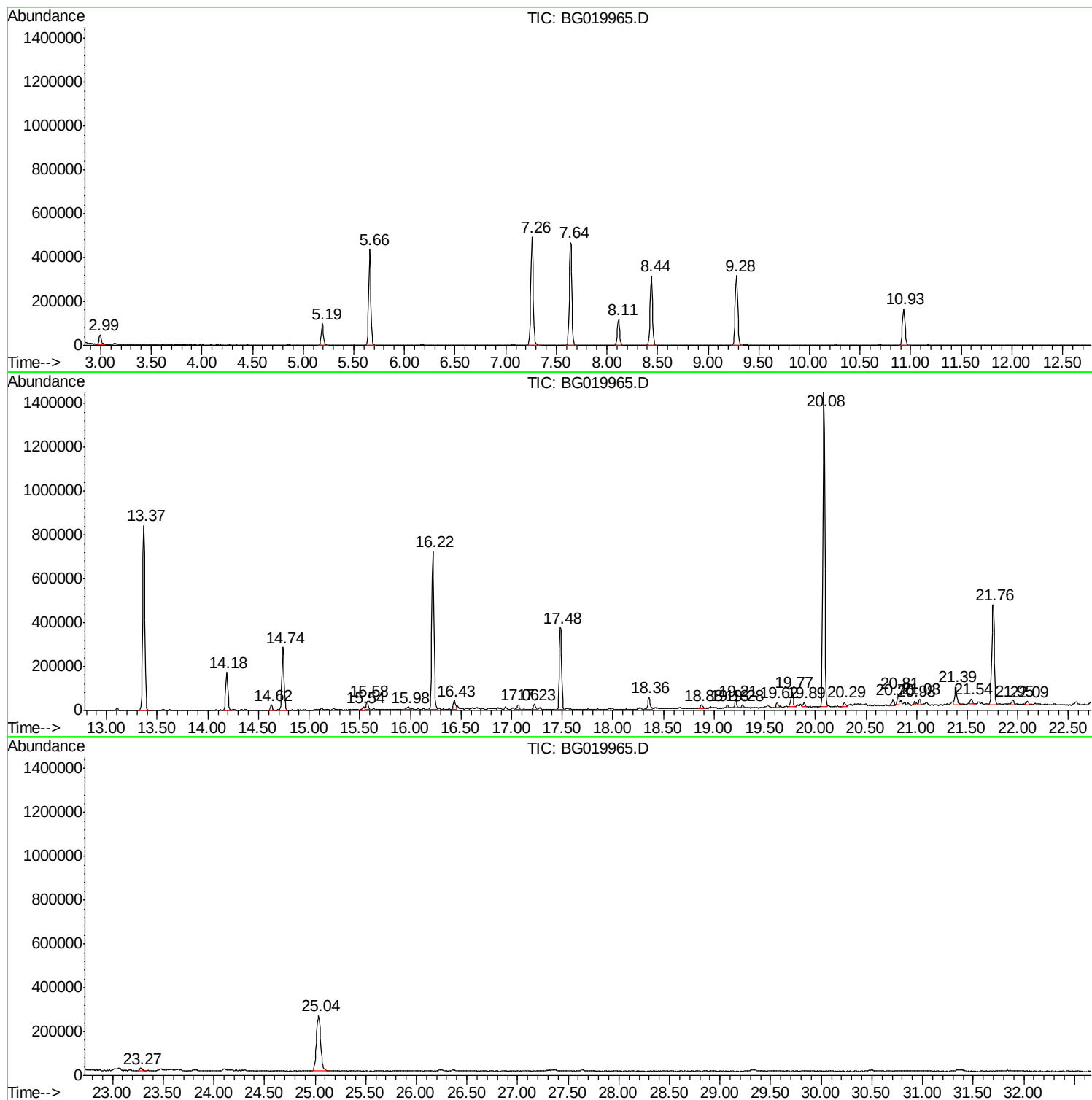
Sum of corrected areas: 12290891

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

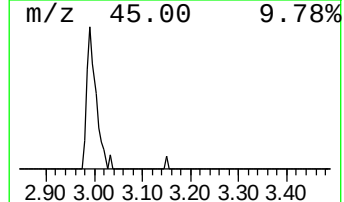
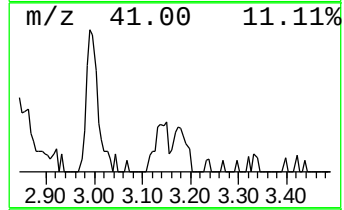
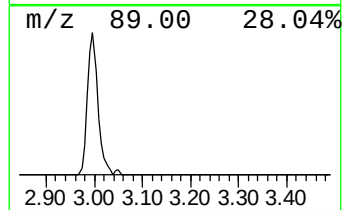
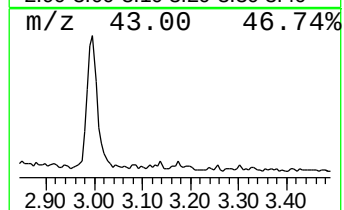
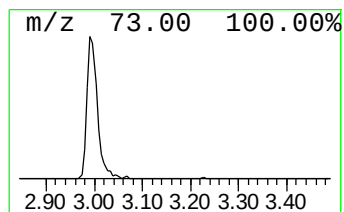
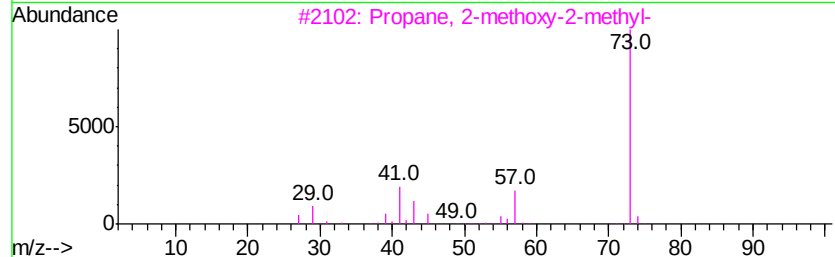
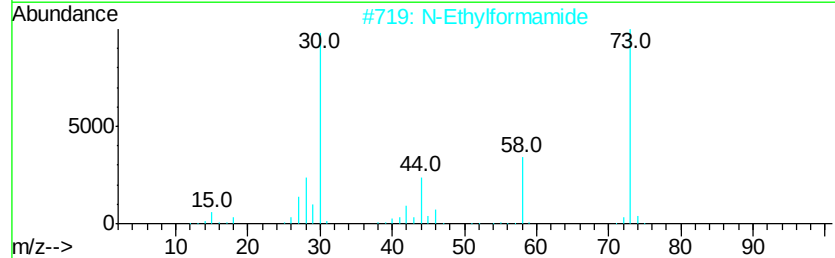
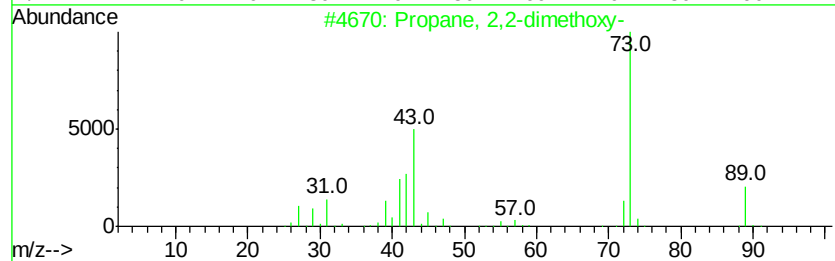
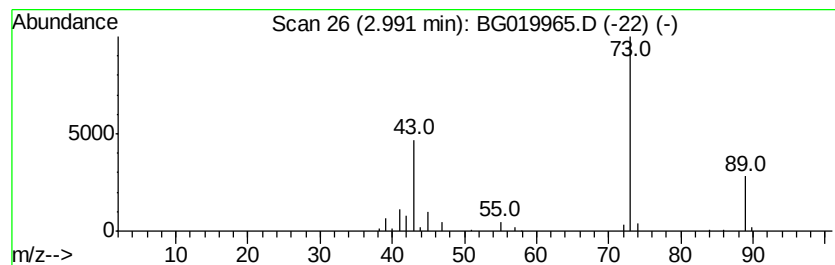
Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.99	6.43 ng	62506	1,4-Dichlorobenzene-d4	8.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	.beta.-Alanine	89	C3H7NO2	000107-95-9	5



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

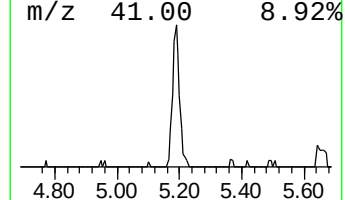
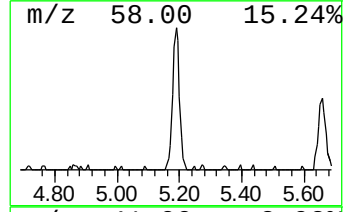
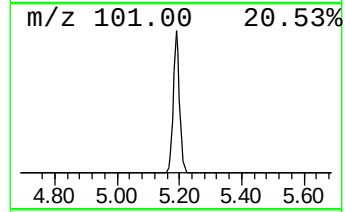
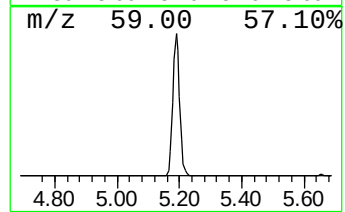
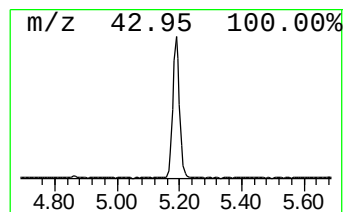
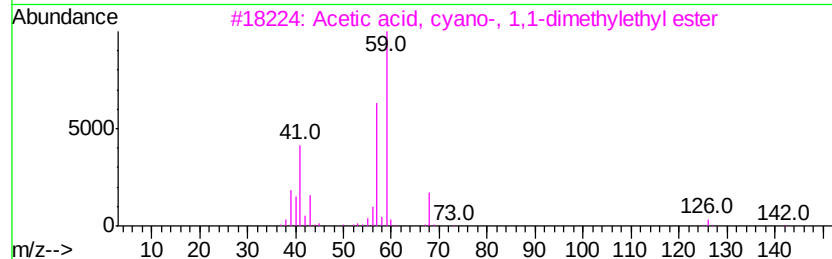
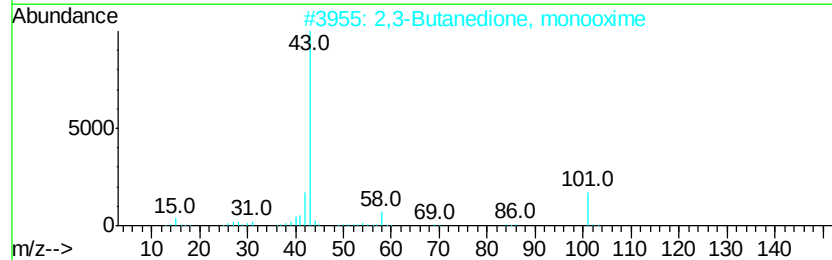
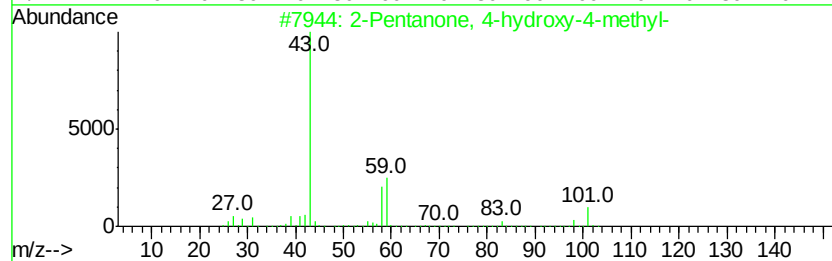
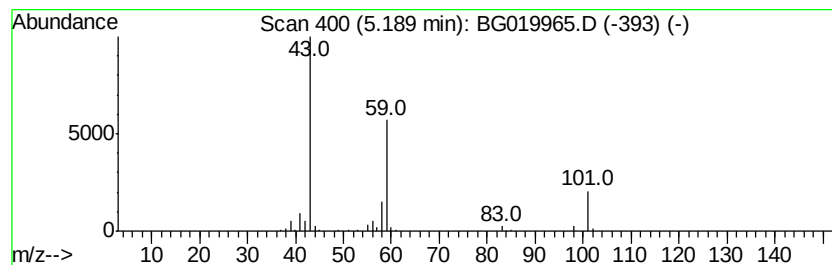
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	15.65 ng	152189	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Heptanol	116	C7H16O	000589-82-2	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

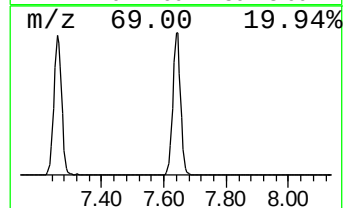
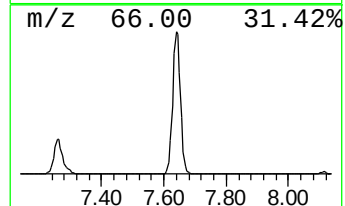
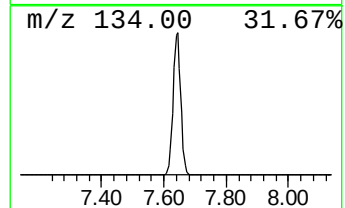
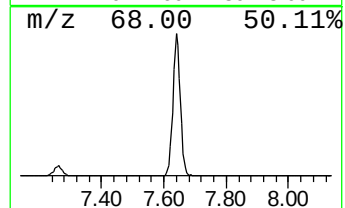
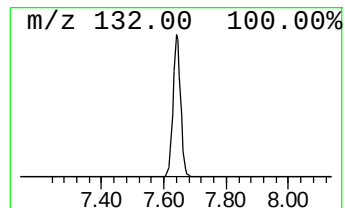
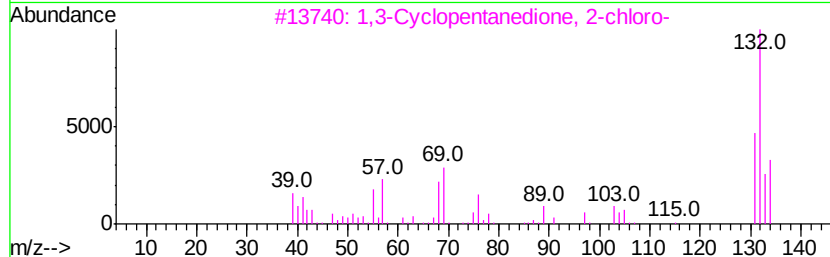
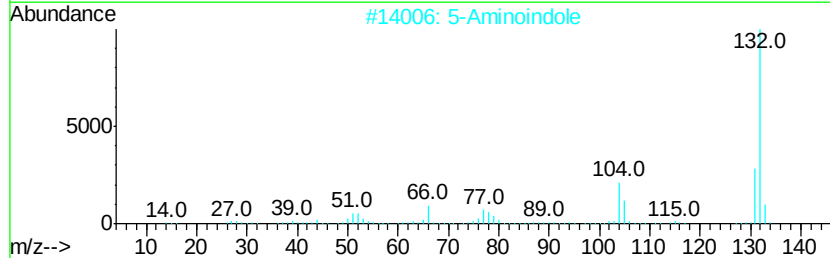
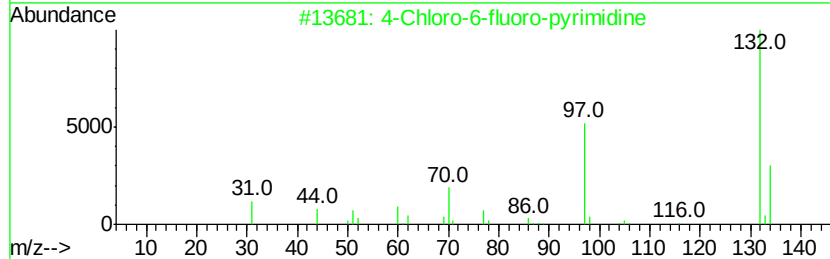
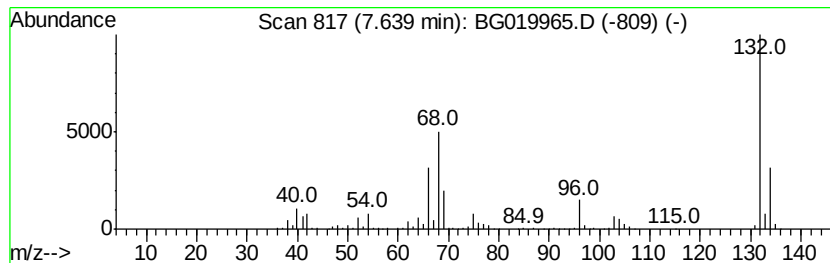
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	82.98 ng	807072	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

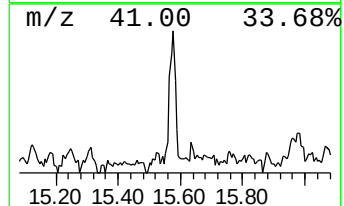
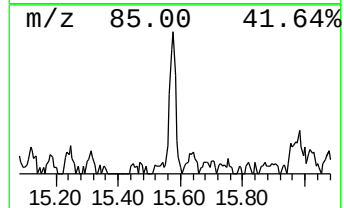
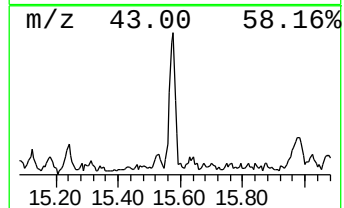
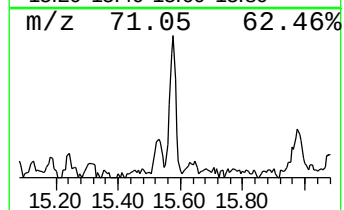
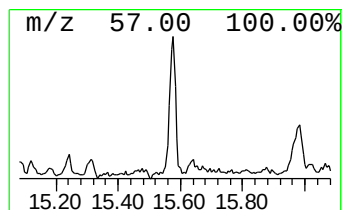
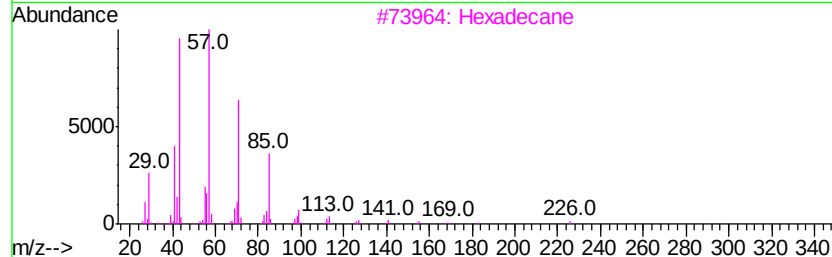
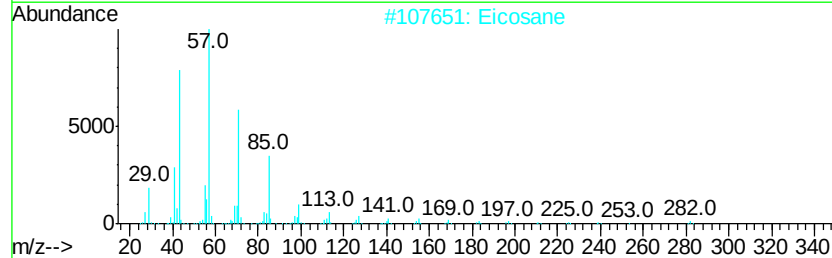
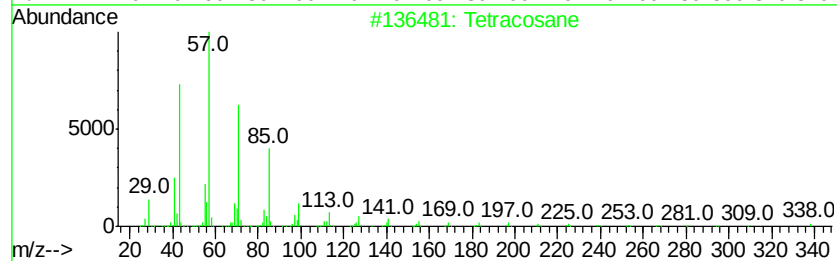
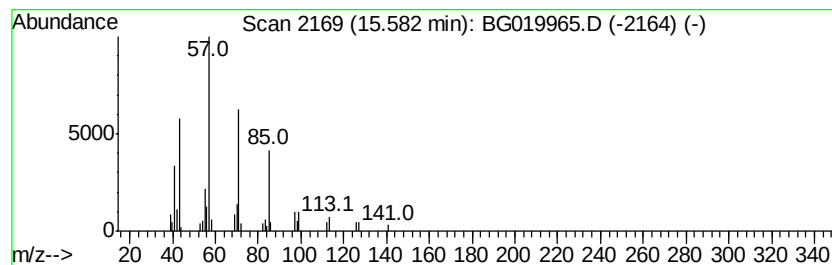
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.34 ng	53566	Acenaphthene-d10	14.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	90
2		Eicosane	282	C20H42	000112-95-8	86
3		Hexadecane	226	C16H34	000544-76-3	78
4		Heptadecane	240	C17H36	000629-78-7	78
5		Pentadecane	212	C15H32	000629-62-9	78



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

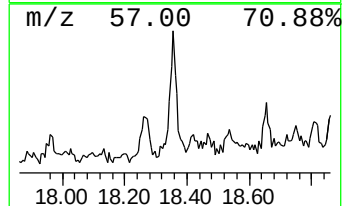
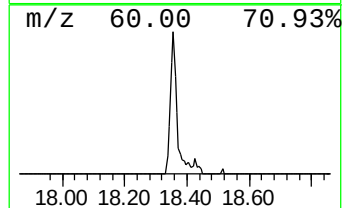
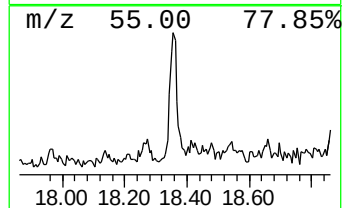
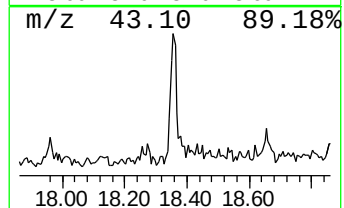
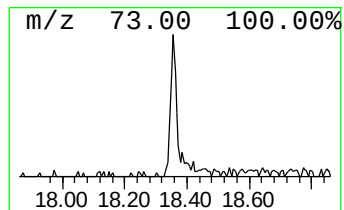
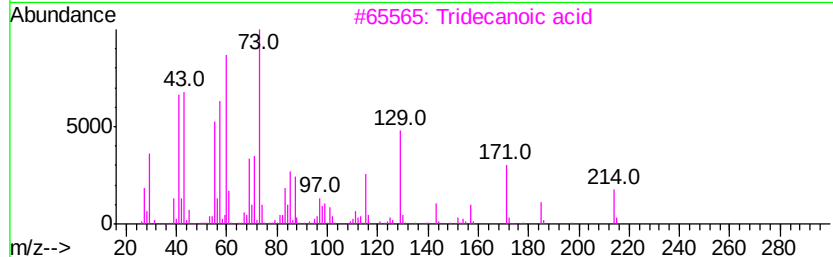
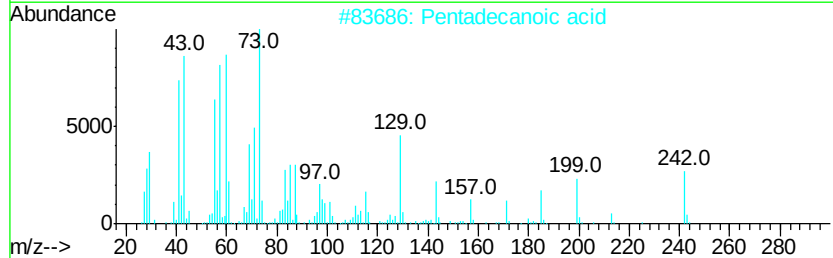
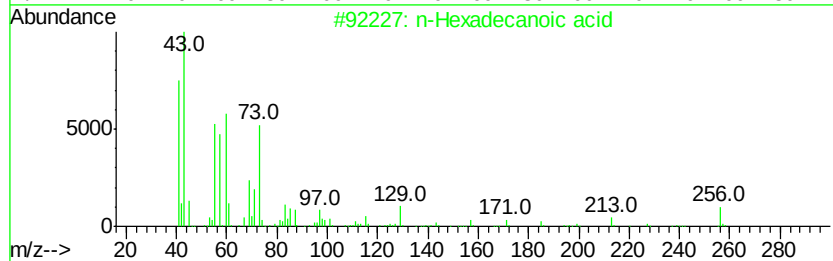
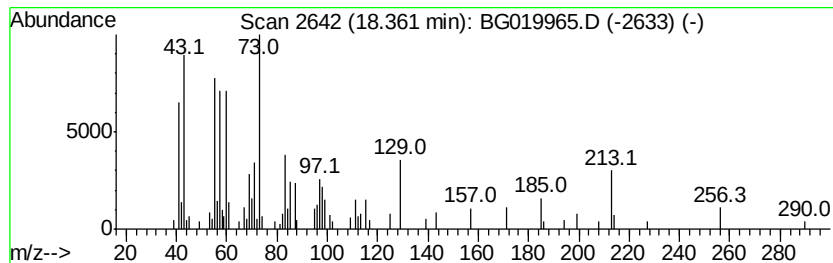
Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.36	2.73 ng	81576	Phenanthrene-d10	17.48		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3		Tridecanoic acid	214	C13H26O2	000638-53-9	59
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

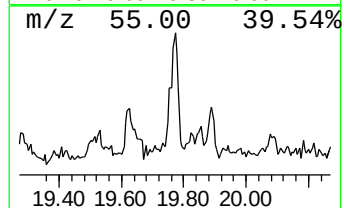
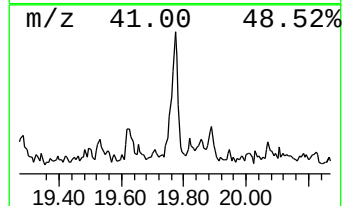
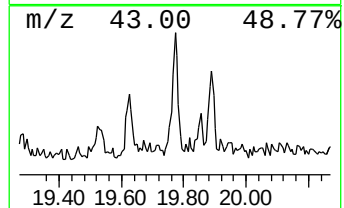
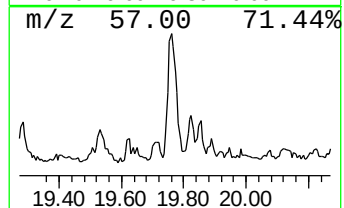
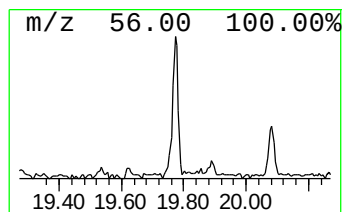
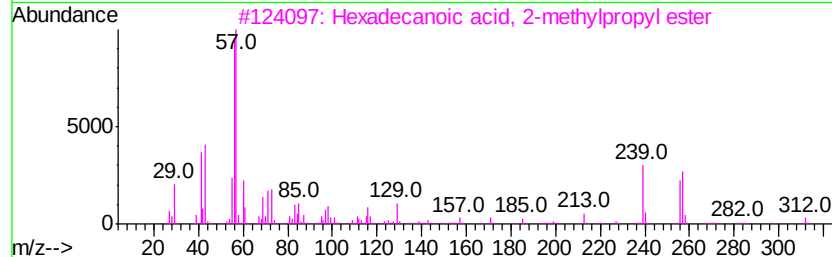
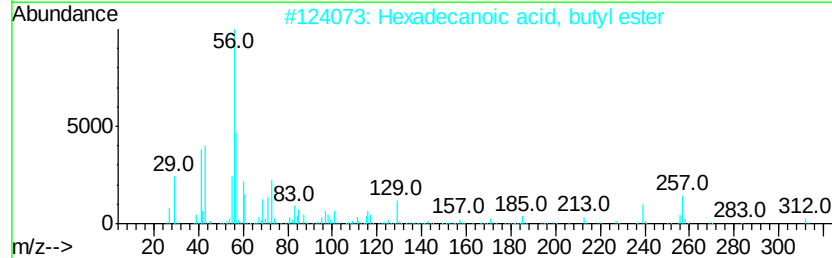
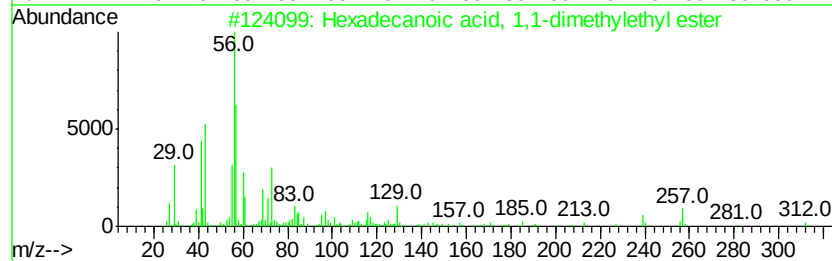
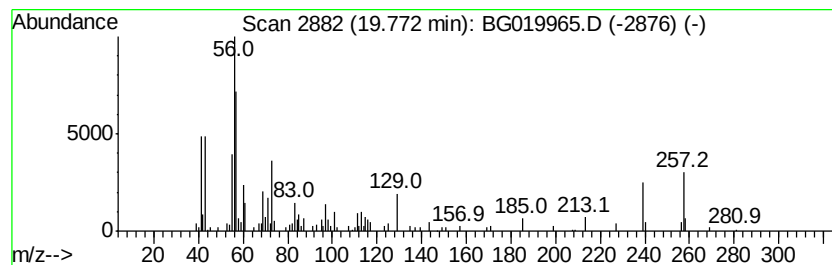
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.98 ng	114559	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
4		2-Methyl-1-octadecene	266	C19H38	061868-20-0	30
5		Cycloheptylamine	113	C7H15N	005452-35-7	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

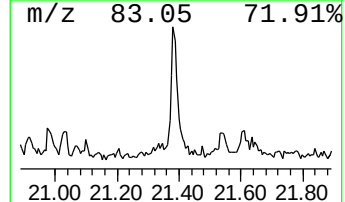
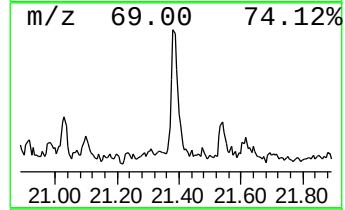
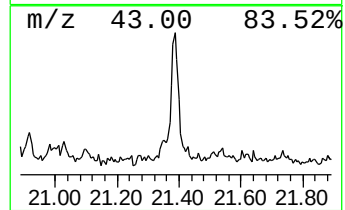
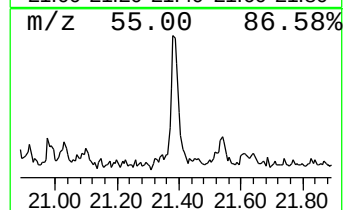
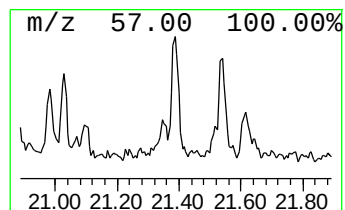
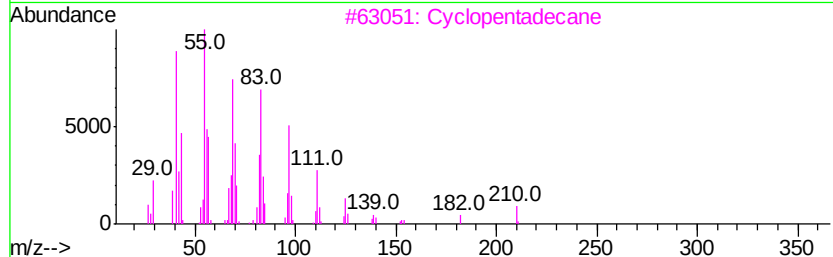
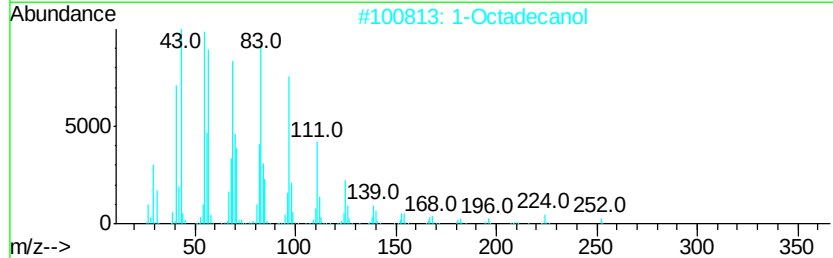
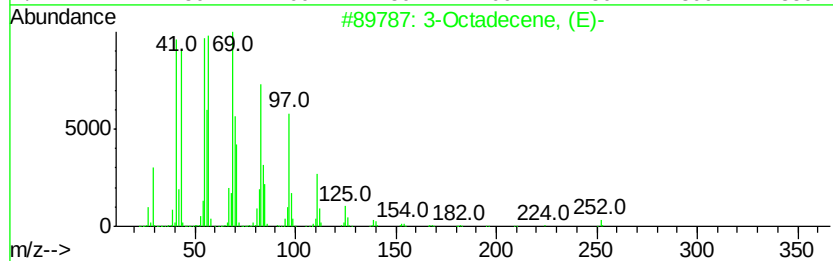
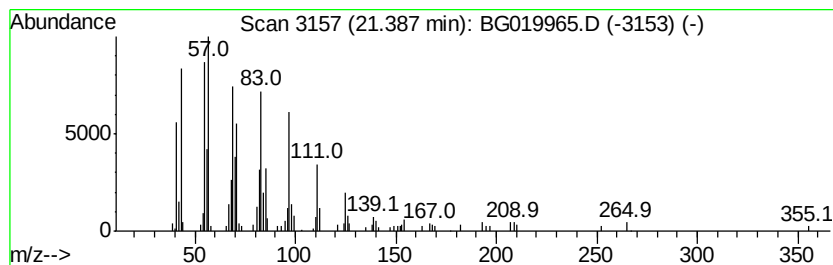
Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.39	3.32 ng	127551	Chrysene-d12	21.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	94
2	1-Octadecanol	270	C18H38O	000112-92-5	93
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	93
5	Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019965.D
Acq On : 6 Dec 2015 13:50
Operator : UM/NP
Sample : G4650-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
Propane, 2,2-dime...	2.99	6.4	ng	62506	1	8.11	194517	20.0
2-Pentanone, 4-hy...	5.19	15.7	ng	152189	1	8.11	194517	20.0
unknown7.64	7.64	83.0	ng	807072	1	8.11	194517	20.0
Tetracosane	15.58	2.3	ng	53566	3	14.74	457531	20.0
n-Hexadecanoic acid	18.36	2.7	ng	81576	4	17.48	596738	20.0
Hexadecanoic acid...	19.77	3.0	ng	114559	5	21.76	769321	20.0
3-Octadecene, (E)-	21.39	3.3	ng	127551	5	21.76	769321	20.0