

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
 Data File : BG033605.D
 Acq On : 5 Apr 2018 22:56
 Operator : SJ/JU
 Sample : J2265-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PF-7

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	3.476	25	32	42	rBV	61617	120503	4.59%	0.847%
2	3.564	43	47	53	rVB	34691	49508	1.88%	0.348%
3	5.767	417	422	429	rBV2	25387	44114	1.68%	0.310%
4	6.284	504	510	527	rBV	437441	912062	34.70%	6.409%
5	7.970	791	797	827	rBV	491932	1167883	44.44%	8.206%
6	8.370	858	865	890	rBV	461014	1047207	39.85%	7.358%
7	8.863	942	949	965	rBV	81148	192172	7.31%	1.350%
8	9.192	998	1005	1024	rBV	343726	701444	26.69%	4.929%
9	10.062	1146	1153	1165	rBV	273114	632972	24.08%	4.448%
10	11.742	1429	1439	1451	rBV	144519	311121	11.84%	2.186%
11	14.104	1834	1841	1861	rBV	862051	1562691	59.46%	10.980%
12	14.898	1970	1976	1985	rBV	70552	120223	4.57%	0.845%
13	15.473	2066	2074	2086	rBV3	304400	550121	20.93%	3.865%
14	16.243	2200	2205	2211	rVB2	37846	48294	1.84%	0.339%
15	16.948	2318	2325	2342	rBV	881014	1497816	56.99%	10.525%
16	17.095	2345	2350	2361	rVB2	39584	73913	2.81%	0.519%
17	18.205	2531	2539	2551	rBV2	418015	725599	27.61%	5.098%
18	19.005	2671	2675	2682	rBV3	56361	88486	3.37%	0.622%
19	20.726	2962	2968	2985	rBV	1882220	2628152	100.00%	18.467%
20	22.066	3191	3196	3204	rBV5	43172	84577	3.22%	0.594%
21	22.553	3270	3279	3293	rBV2	380351	799269	30.41%	5.616%
22	24.416	3588	3596	3606	rVB2	56260	135977	5.17%	0.955%
23	26.319	3907	3920	3938	rBV3	200030	737537	28.06%	5.182%

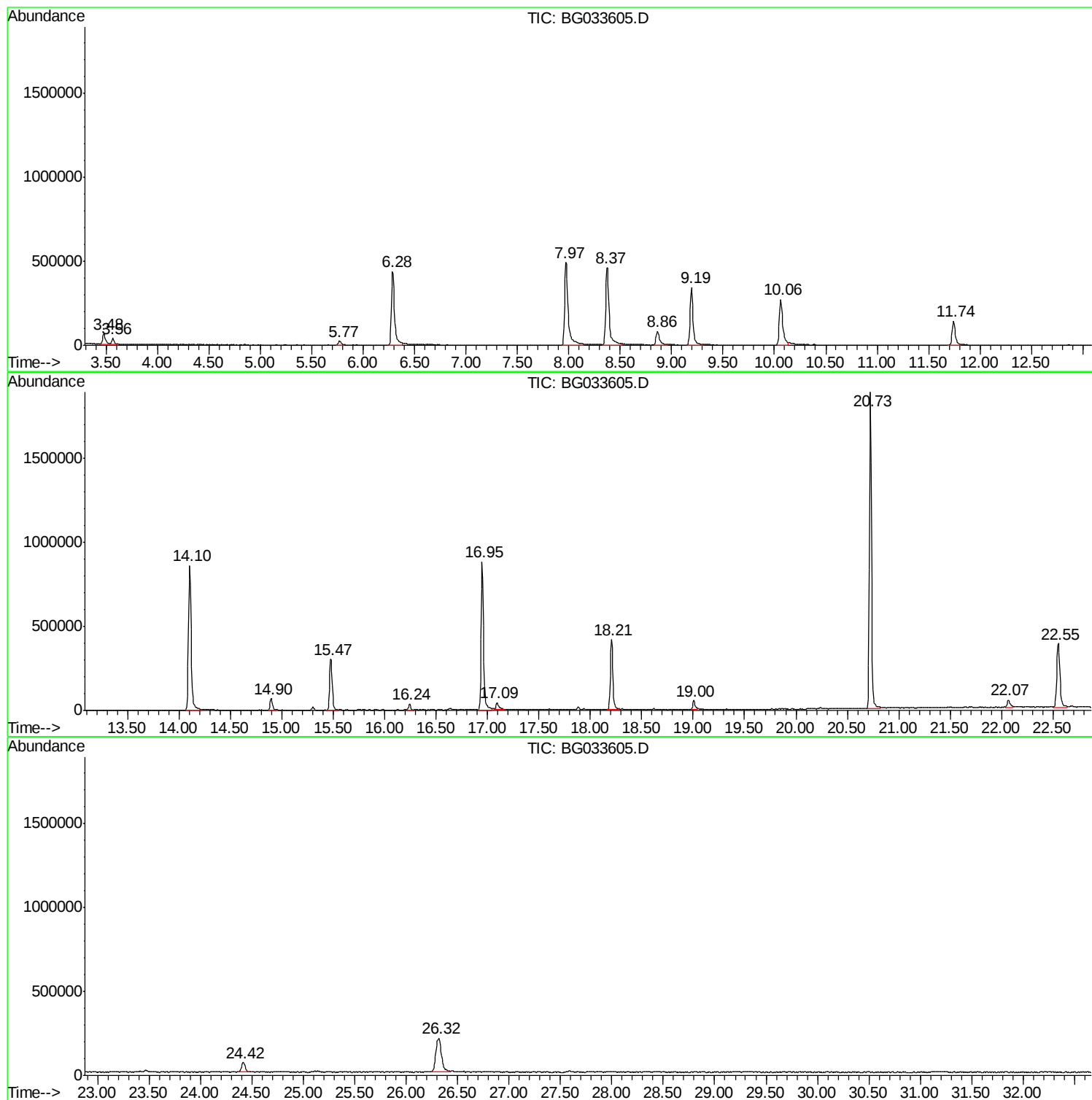
Sum of corrected areas: 14231641

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

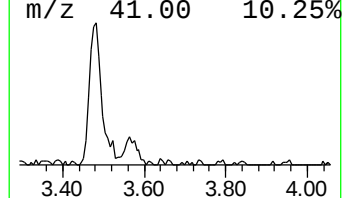
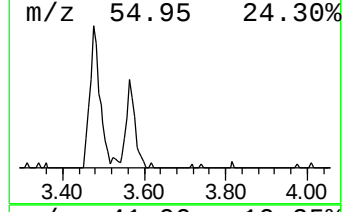
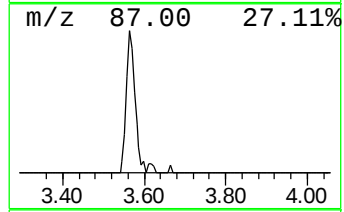
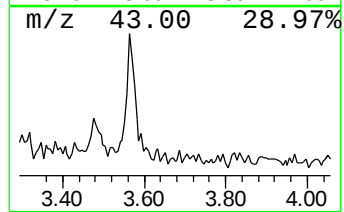
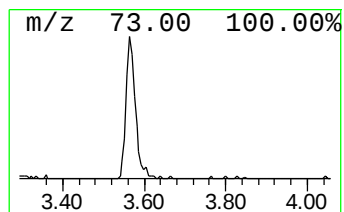
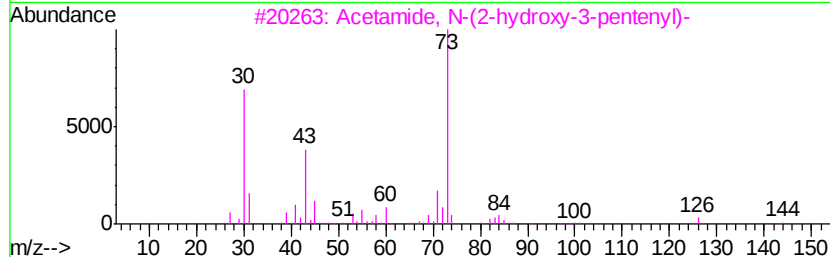
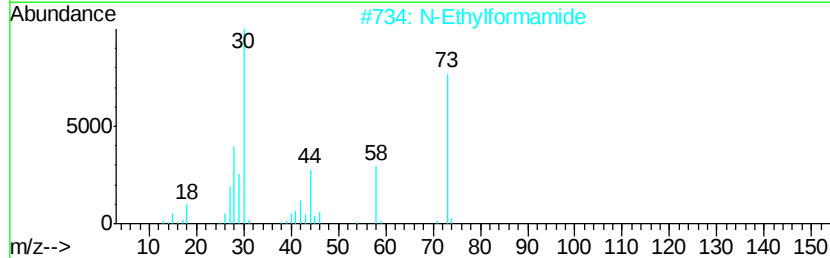
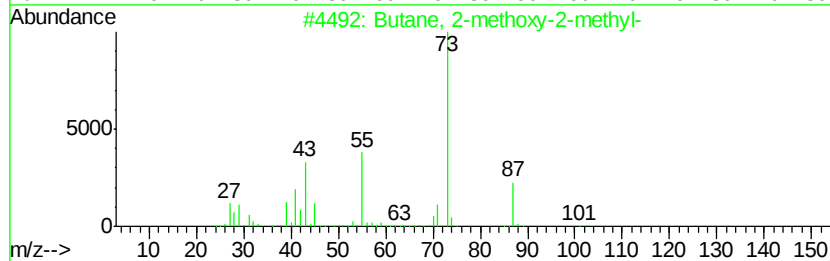
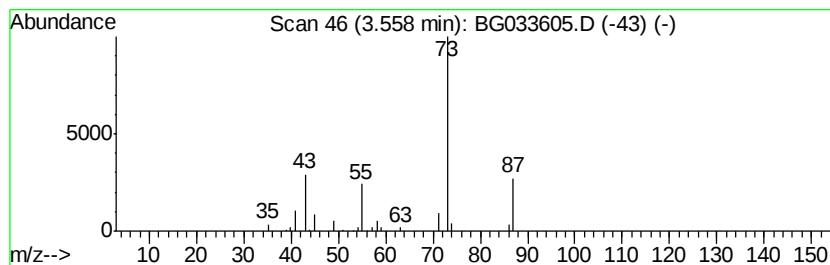
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	5.15 ng	49508	1,4-Dichlorobenzene-d4	8.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

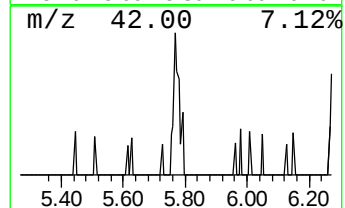
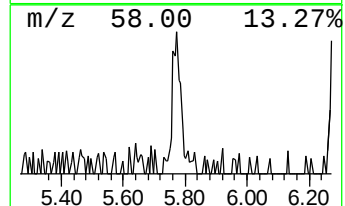
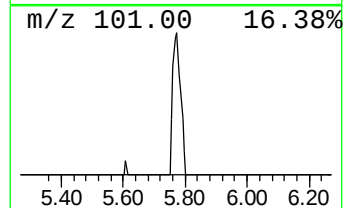
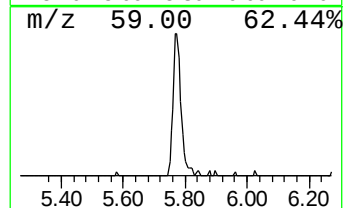
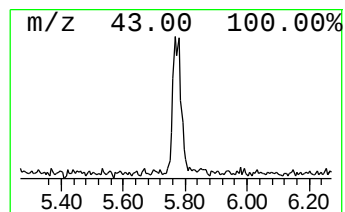
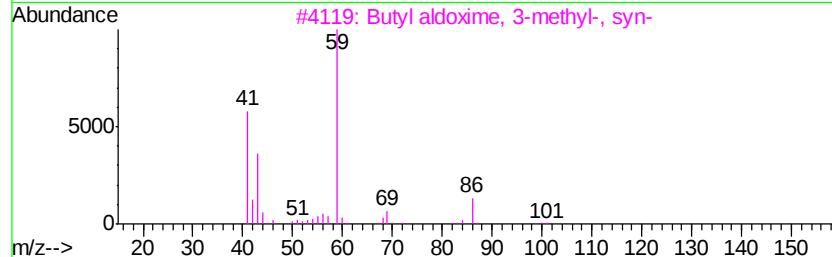
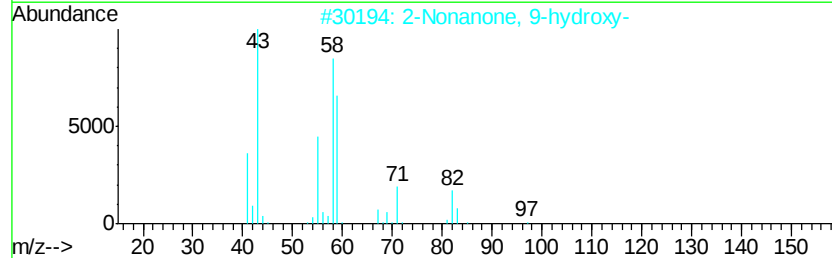
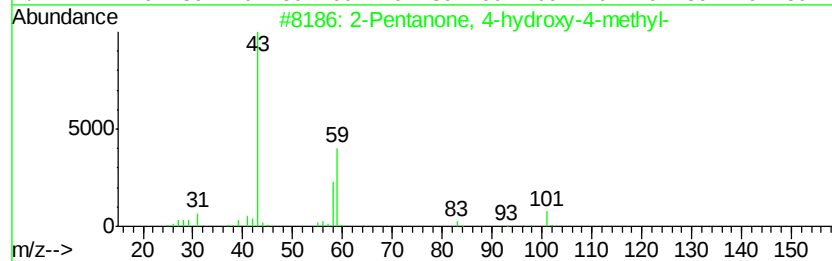
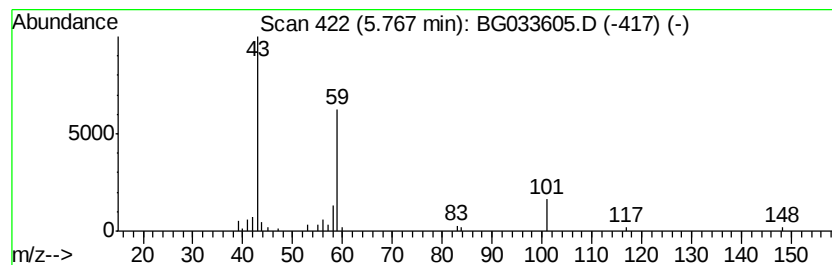
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	4.59 ng	44114	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4		Propane-1,1-diol diacetate	160	C7H12O4	033931-80-5	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

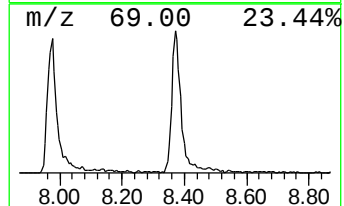
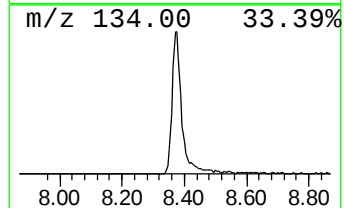
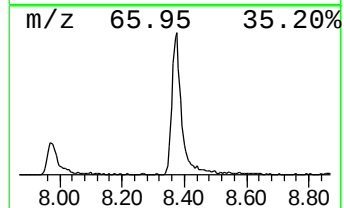
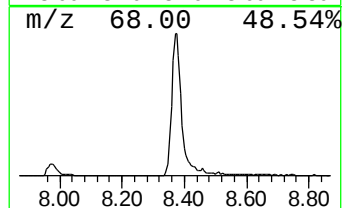
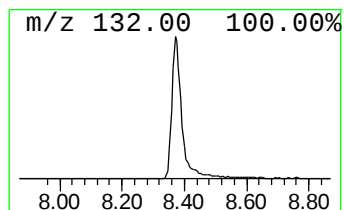
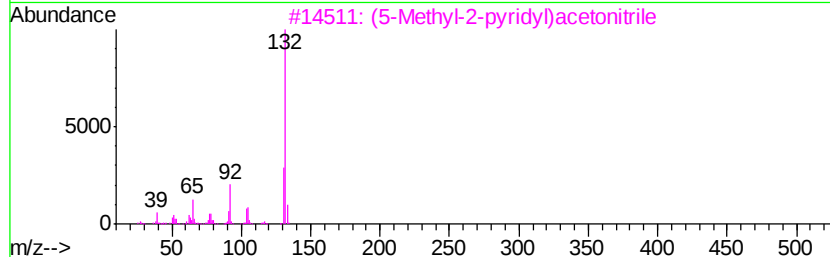
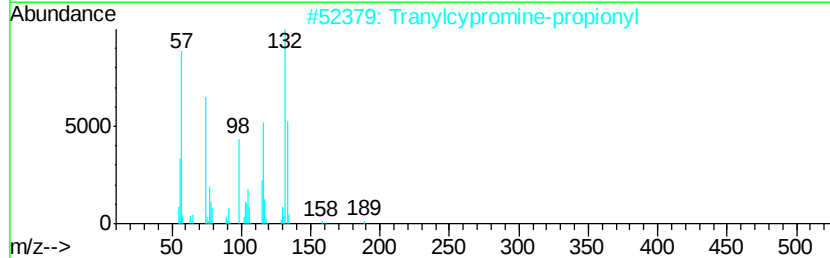
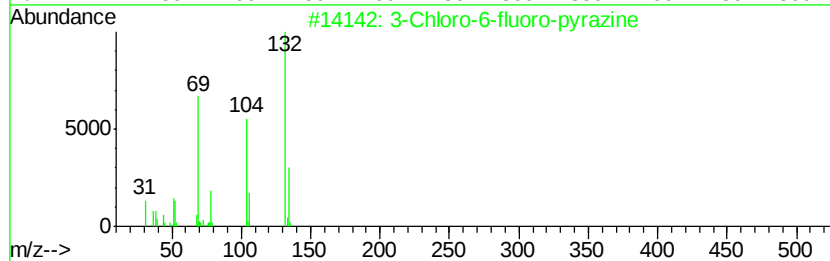
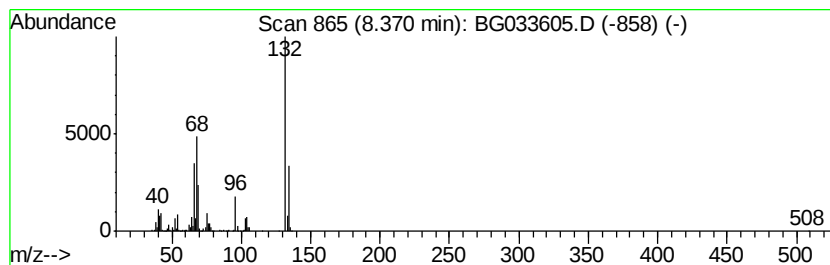
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown8.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	108.99 ng	1047210	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

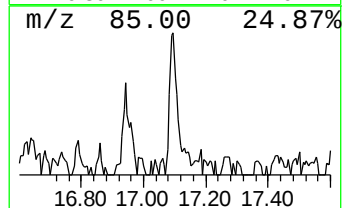
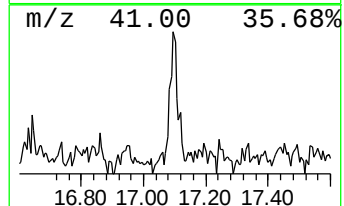
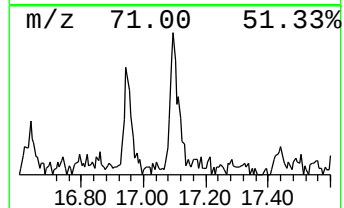
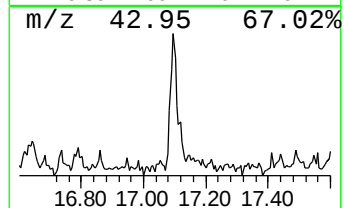
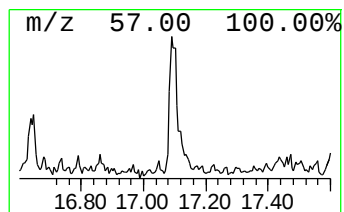
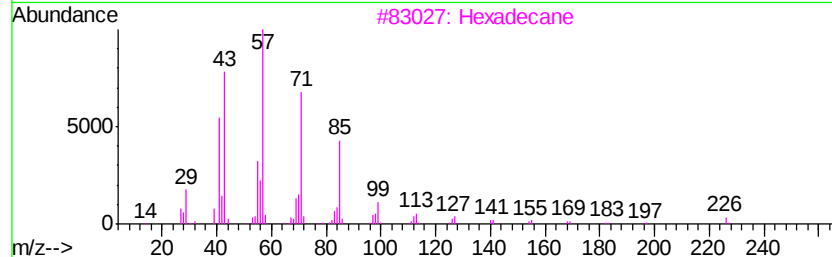
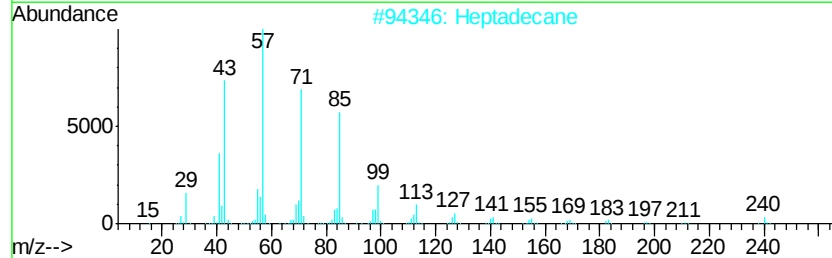
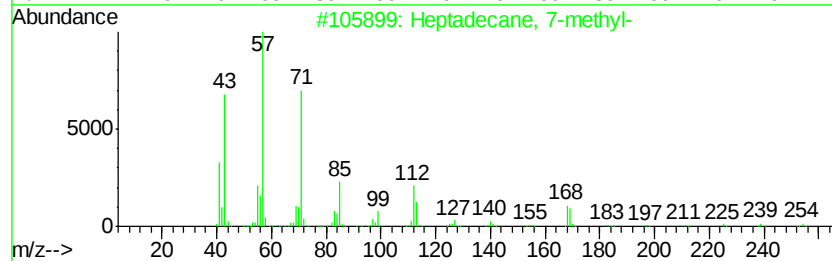
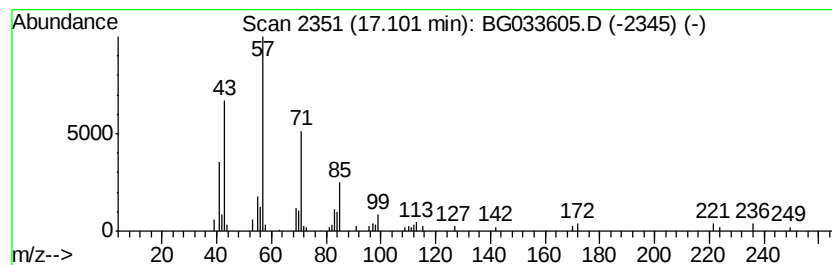
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 7-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.10	2.04 ng	73913	Phenanthrene-d10		18.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	87
2			Heptadecane	240	C17H36	000629-78-7	87
3			Hexadecane	226	C16H34	000544-76-3	72
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

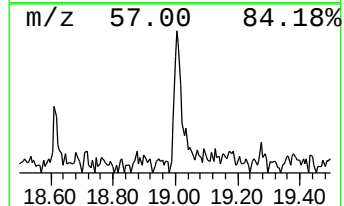
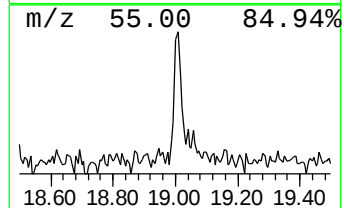
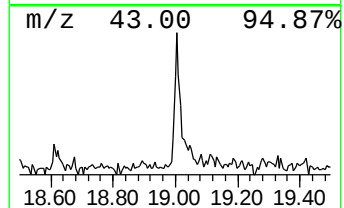
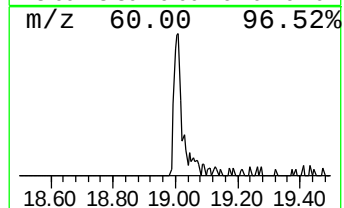
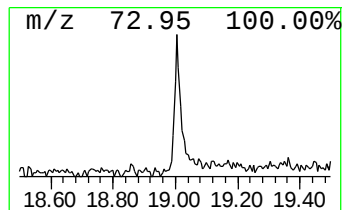
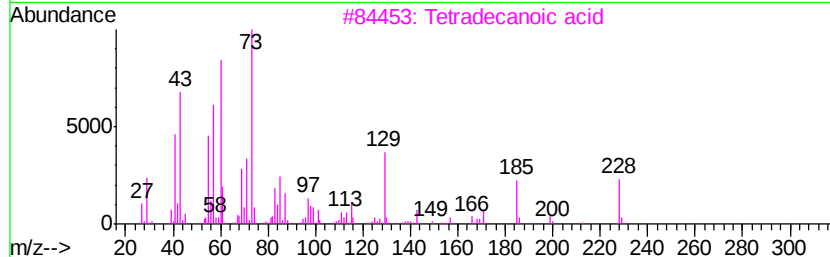
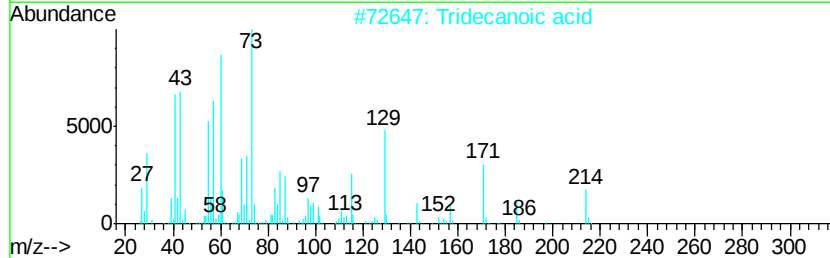
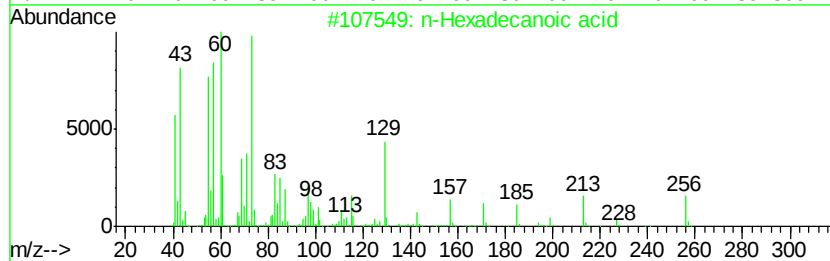
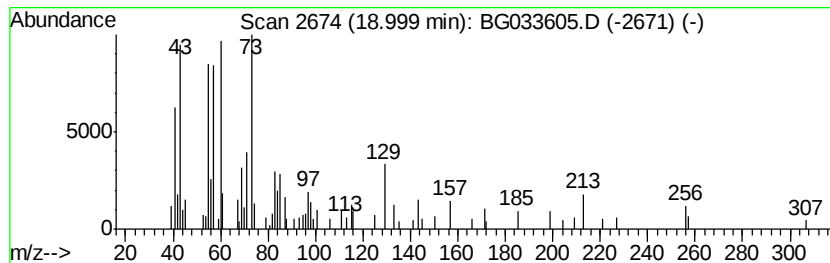
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	2.44 ng	88486	Phenanthrene-d10	18.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

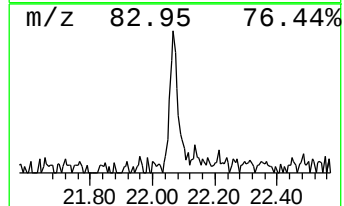
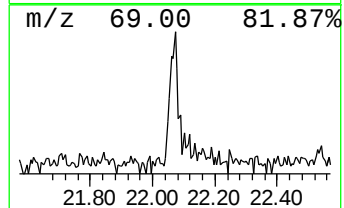
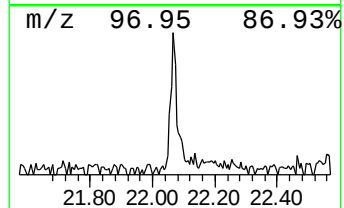
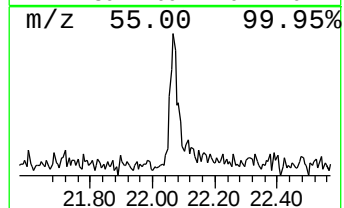
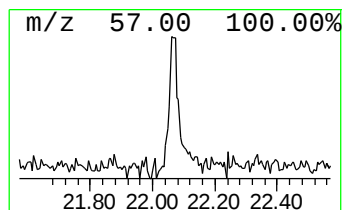
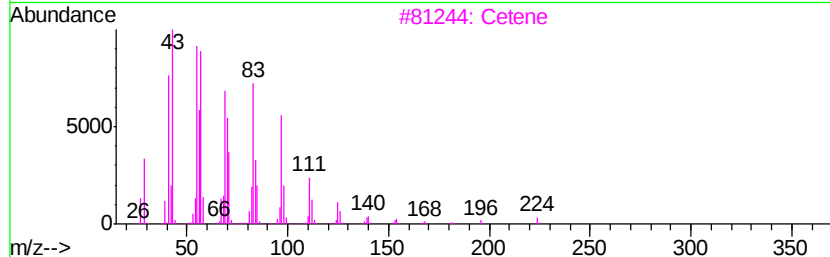
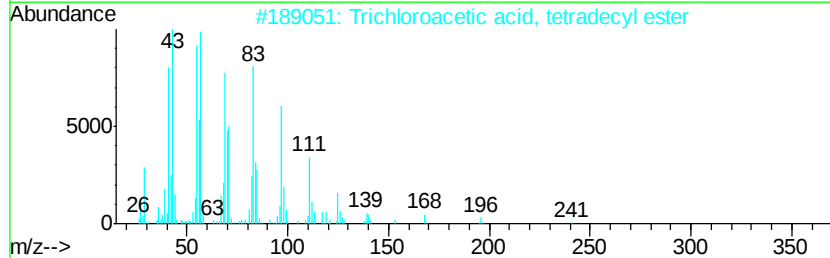
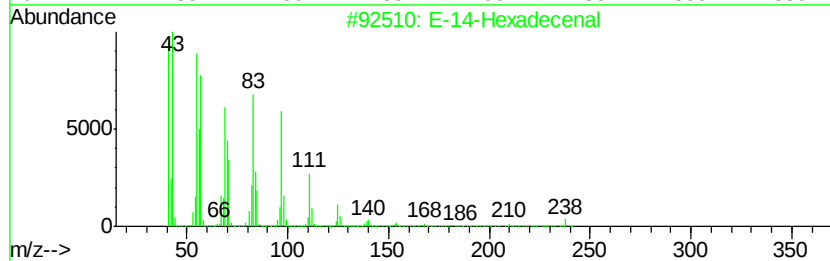
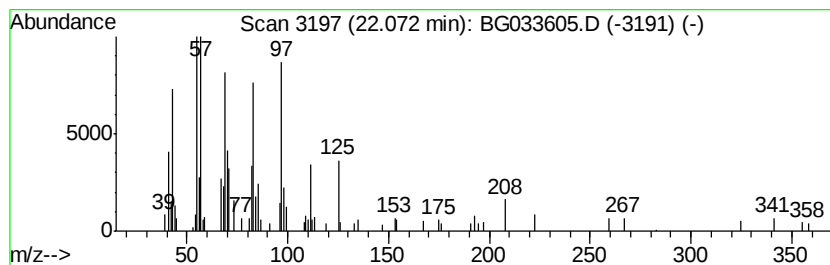
Instrument :
BNA_G
ClientSampleId :
PF-7

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 8 E-14-Hexadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.12 ng	84577	Chrysene-d12	22.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9 95
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9 93
3	Cetene	224	C16H32	000629-73-2 89
4	8-Heptadecene	238	C17H34	002579-04-6 89
5	1-Heneicosanol	312	C21H44O	015594-90-8 81



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

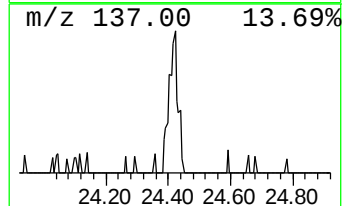
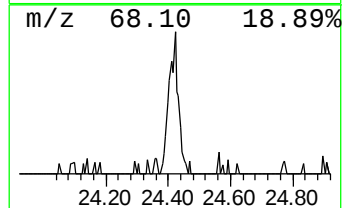
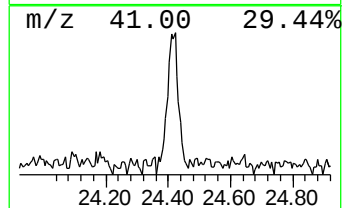
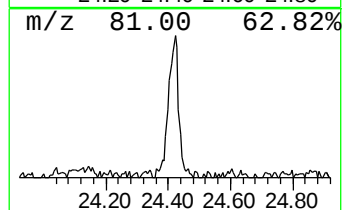
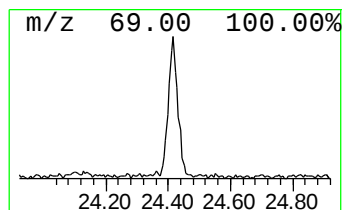
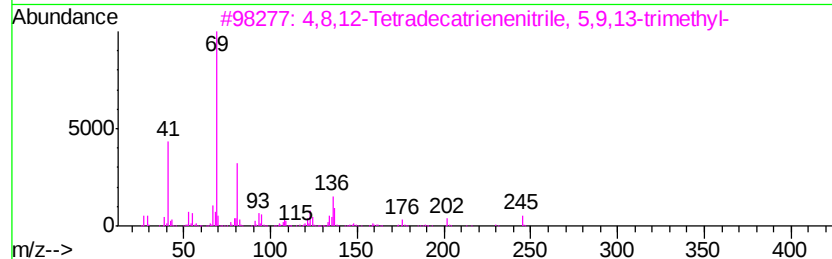
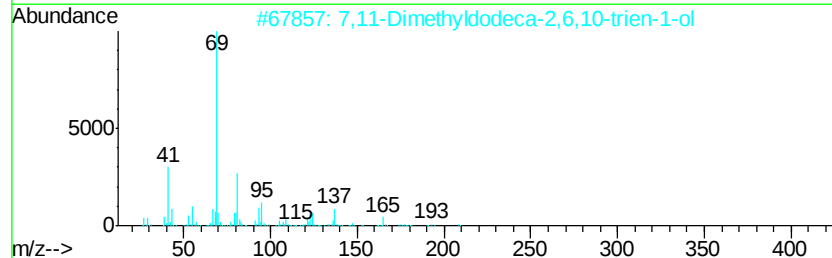
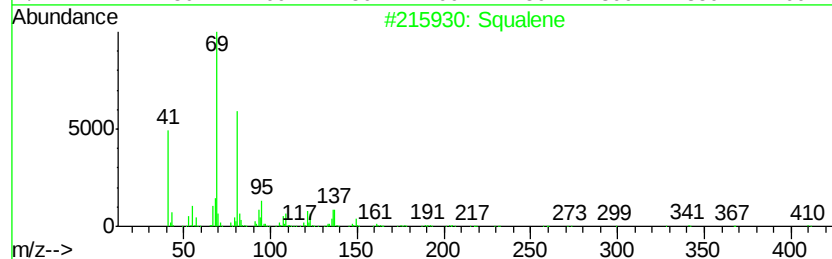
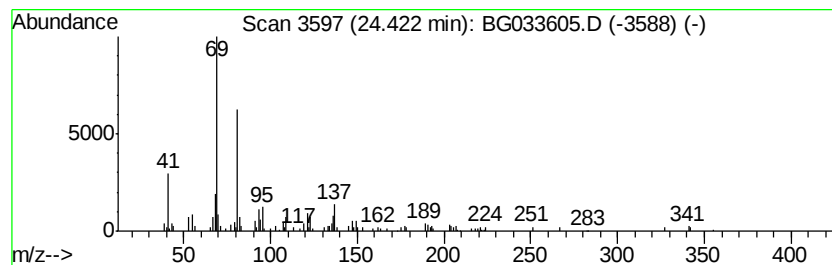
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.42	3.40 ng	135977	Chrysene-d12	22.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	72
2		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3		4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	56
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	56



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040518\
Data File : BG033605.D
Acq On : 5 Apr 2018 22:56
Operator : SJ/JU
Sample : J2265-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PF-7

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
Butane, 2-methoxy...	3.56	5.2	ng	49508	1	8.86	192172	20.0
2-Pentanone, 4-hy...	5.77	4.6	ng	44114	1	8.86	192172	20.0
unknown8.37	8.37	109.0	ng	1047210	1	8.86	192172	20.0
Heptadecane, 7-me...	17.10	2.0	ng	73913	4	18.21	725599	20.0
n-Hexadecanoic acid	19.00	2.4	ng	88486	4	18.21	725599	20.0
E-14-Hexadecenal	22.07	2.1	ng	84577	5	22.55	799269	20.0
Squalene	24.42	3.4	ng	135977	5	22.55	799269	20.0