LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012018\
Data File : BG032195.D
Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

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-BG011218.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	5.666	397	405	413	rBV	32756	54509	1.52%	0.301%
2	6.177	484	492	502	rBV	608212	1080105	30.15%	5.956%
3	7.852	768	777	792	rBV	615994	1192834	33.30%	6.578%
4	8.257	838	846	858	rVB	676831	1224267	34.17%	6.751%
5	8.739	921	928	937	rVB	138209	255446	7.13%	1.409%
6	9.080	976	986	996	rBV	520961	974180	27.19%	5.372%
7	9.938	1124	1132	1142	rBV	375566	698396	19.49%	3.851%
8	11.624	1411	1419	1431	rVB	185379	345820	9.65%	1.907%
9	14.004	1816	1824	1836	rBB	1245145	1948889	54.40%	10.747%
10	14.803	1950	1960	1966	rBV	101322	157585	4.40%	0.869%
11	15.378	2048	2058	2069	rBV2	321389	526497	14.70%	2.903%
12	16.706	2278	2284	2293	rVB	73333	112677	3.15%	0.621%
13	16.853	2302	2309	2320	rBV	1144904	1813375	50.62%	10.000%
14	18.111	2516	2523	2533	rVB2	466162	727923	20.32%	4.014%
15	18.927	2657	2662	2668	rBV3	37698	51822	1.45%	0.286%
16	20.649	2948	2955	2966	rBV	2672692	3582541	100.00%	19.756%
17	21.982	3177	3182	3189	rBV2	75749	116425	3.25%	0.642%
18	22.447	3251	3261	3269	rBV	547649	1022874	28.55%	5.641%
19	24.198	3551	3559	3568	rBV6	19689	49258	1.37%	0.272%
20	25.408	3757	3765	3774	rBV4	35947	105717	2.95%	0.583%
21	26.148	3877	3891	3904	rBV2	321256	1049095	29.28%	5.785%
22	26.912	4009	4021	4039	rVB4	64050	249813	6.97%	1.378%
23	28.780	4322	4339	4356	rBV4	95752	488499	13.64%	2.694%
24	31.136	4724	4740	4741	rBV2	110180	305639	8.53%	1.685%

Sum of corrected areas: 18134186

LSC Report - Integrated Chromatogram

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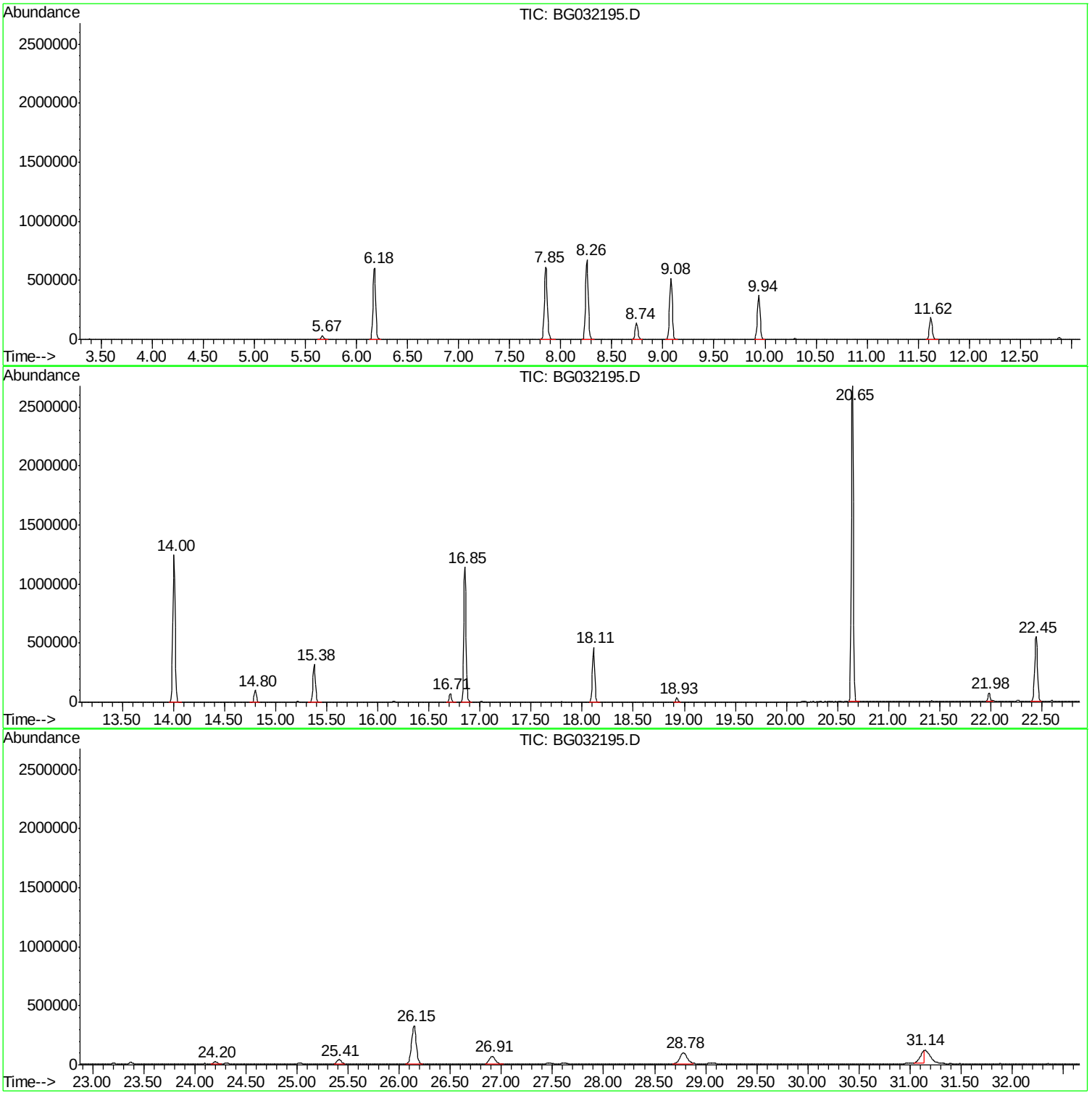
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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\BG012018\
Data File : BG032195.D
Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

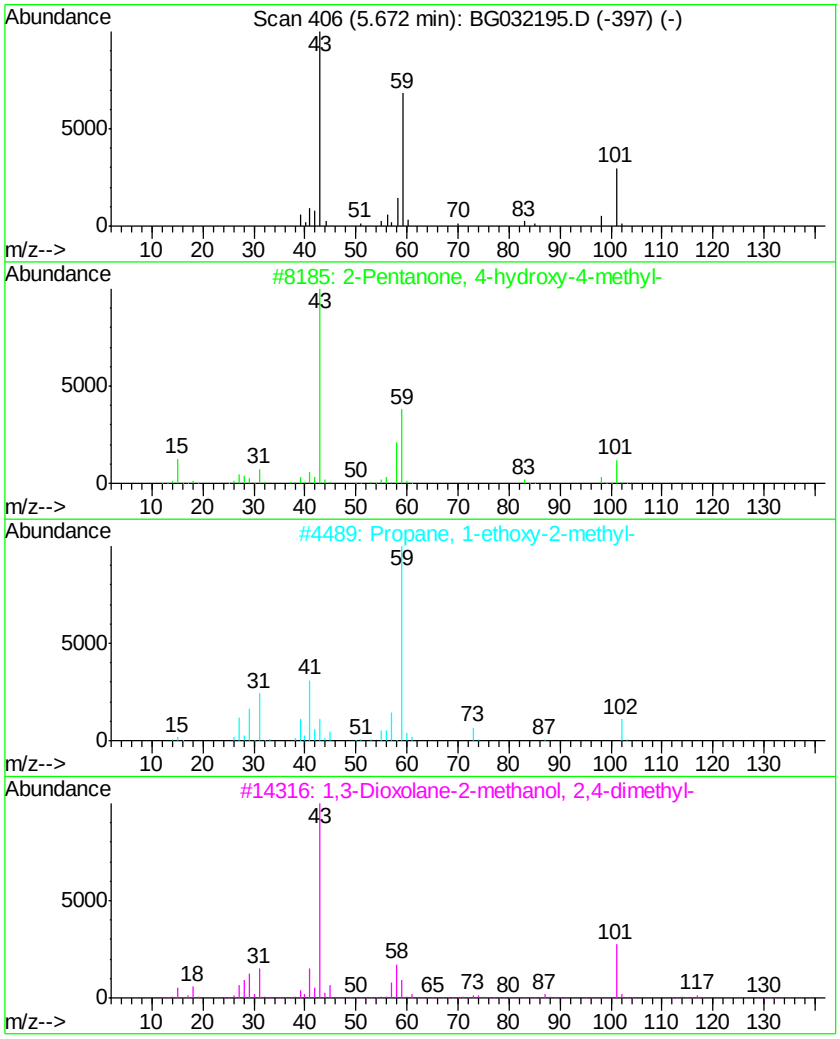
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

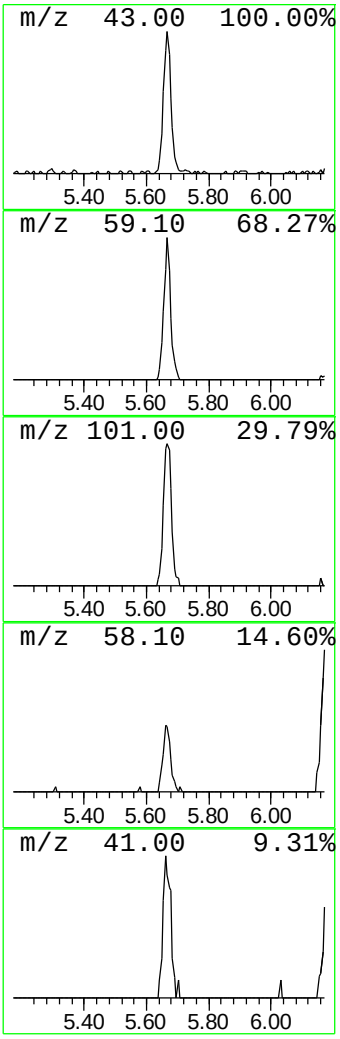
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	4.27 ng	54509	1,4-Dichlorobenzene-d4	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	47
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012018\
Data File : BG032195.D
Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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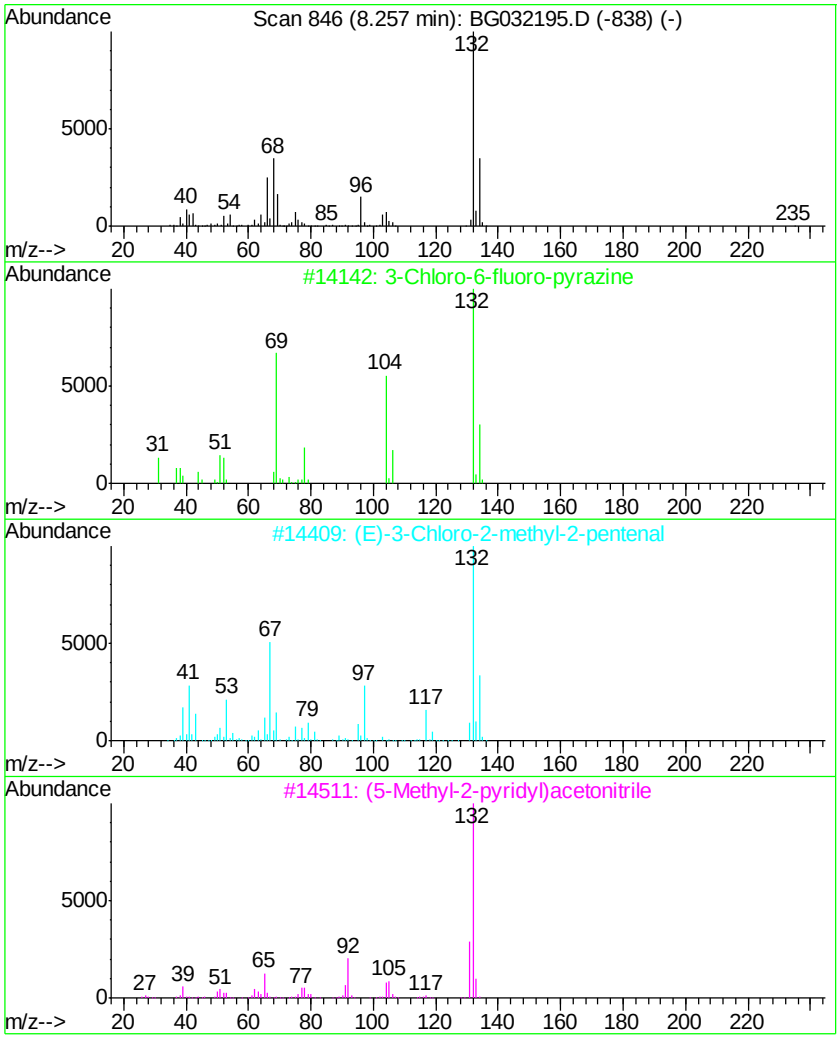
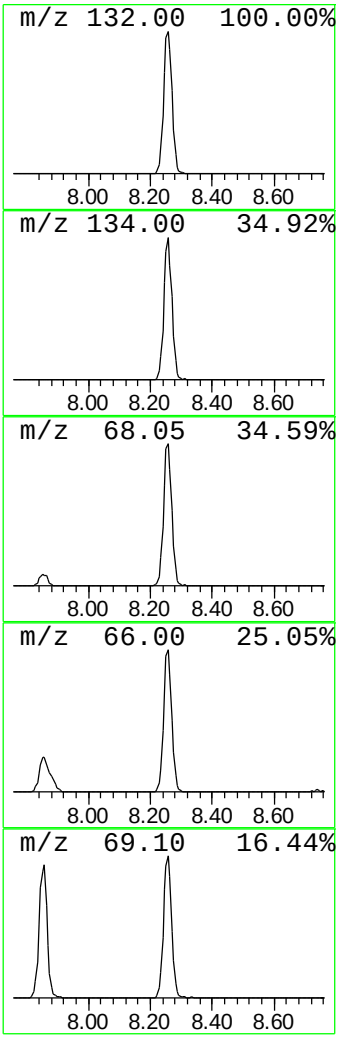
Peak Number 2 unknown8.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	95.85 ng	1224270	1,4-Dichlorobenzene-d4	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012018\
Data File : BG032195.D
Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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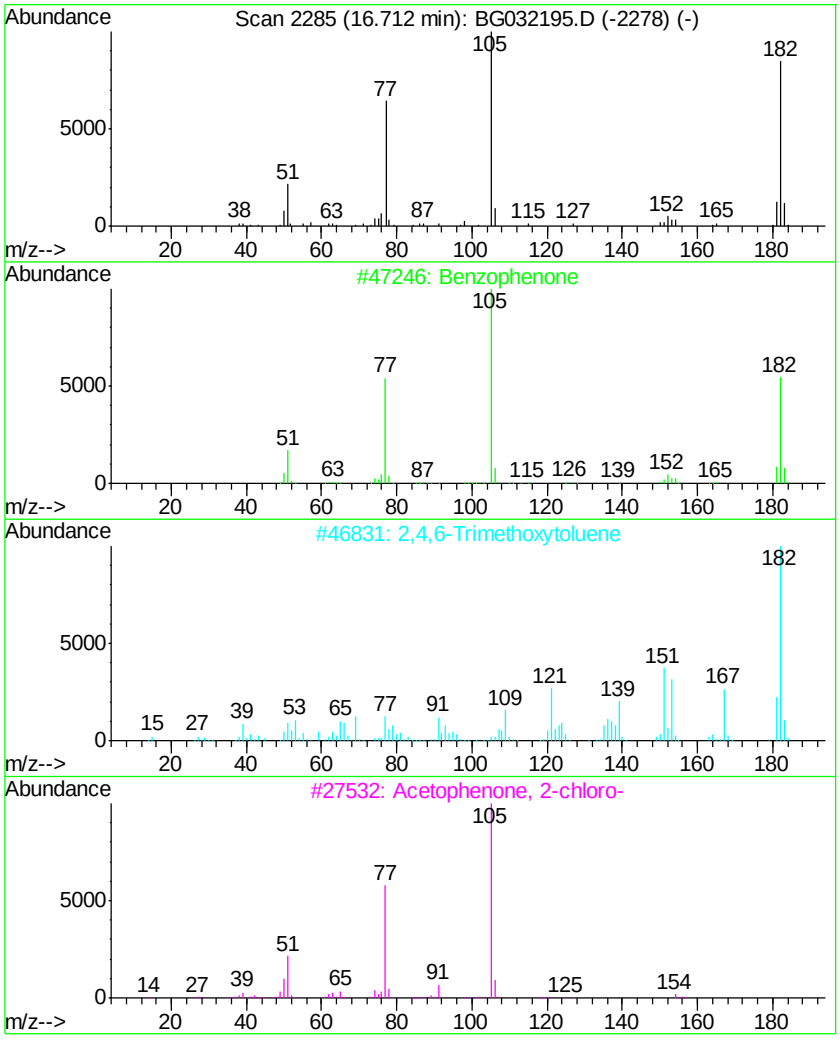
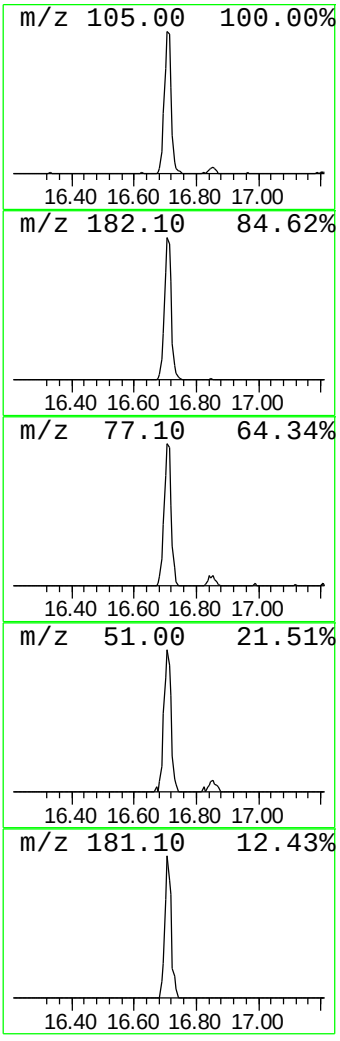
Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	4.28 ng	112677	Acenaphthene-d10	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	38
4	7-Phosphabicyclo[2.2.1]hept-2-en...	182	C11H19P	1000151-83-5	38
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	35





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012018\
Data File : BG032195.D
Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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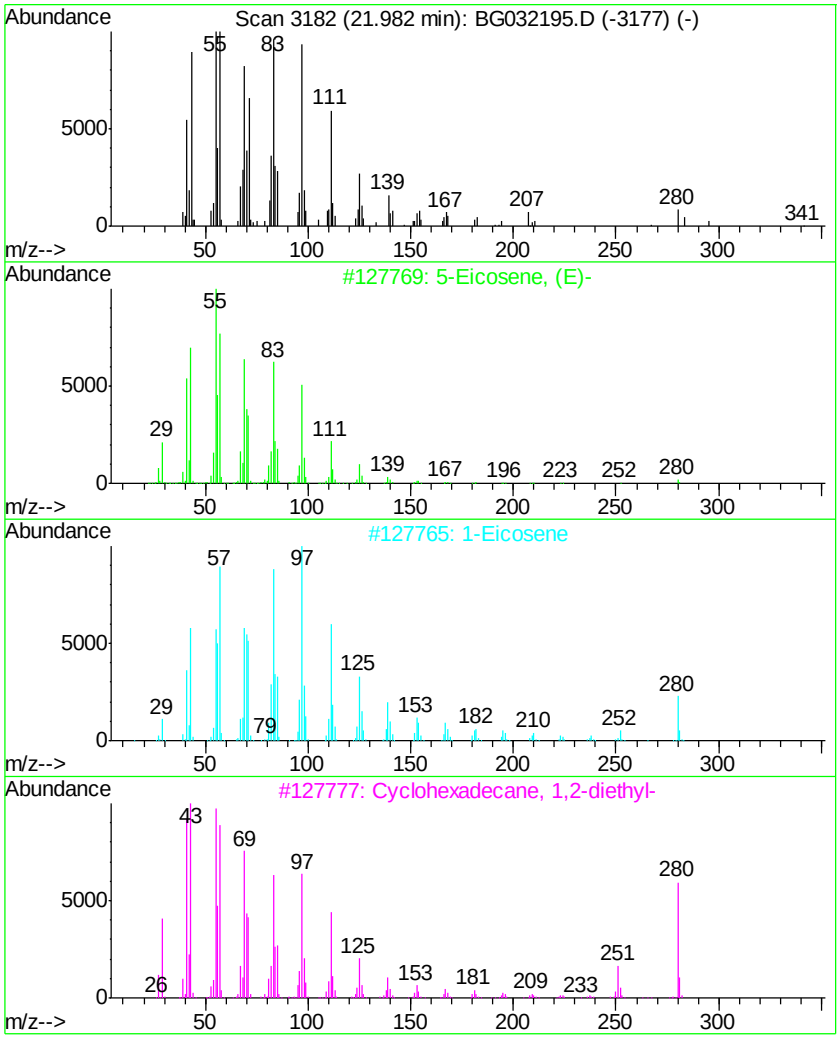
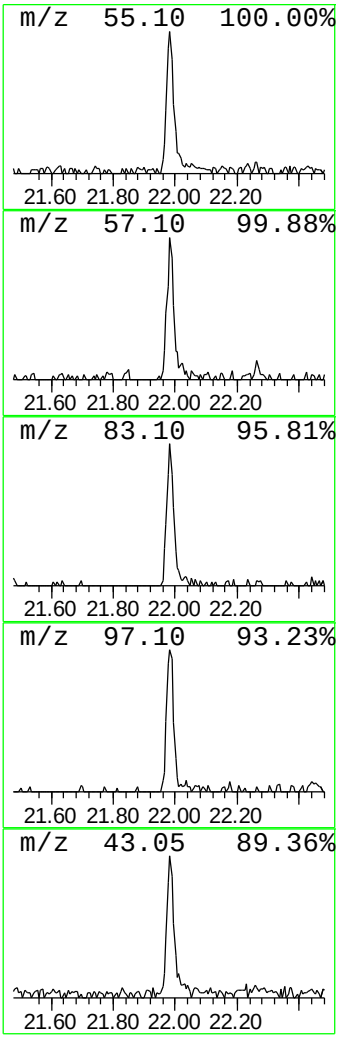
Peak Number 5 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.98	2.28 ng	116425	Chrysene-d12	22.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	1-Eicosene	280	C20H40	003452-07-1	96
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	94





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012018\
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Acq On : 21 Jan 2018 00:57
Operator : SJ/JU
Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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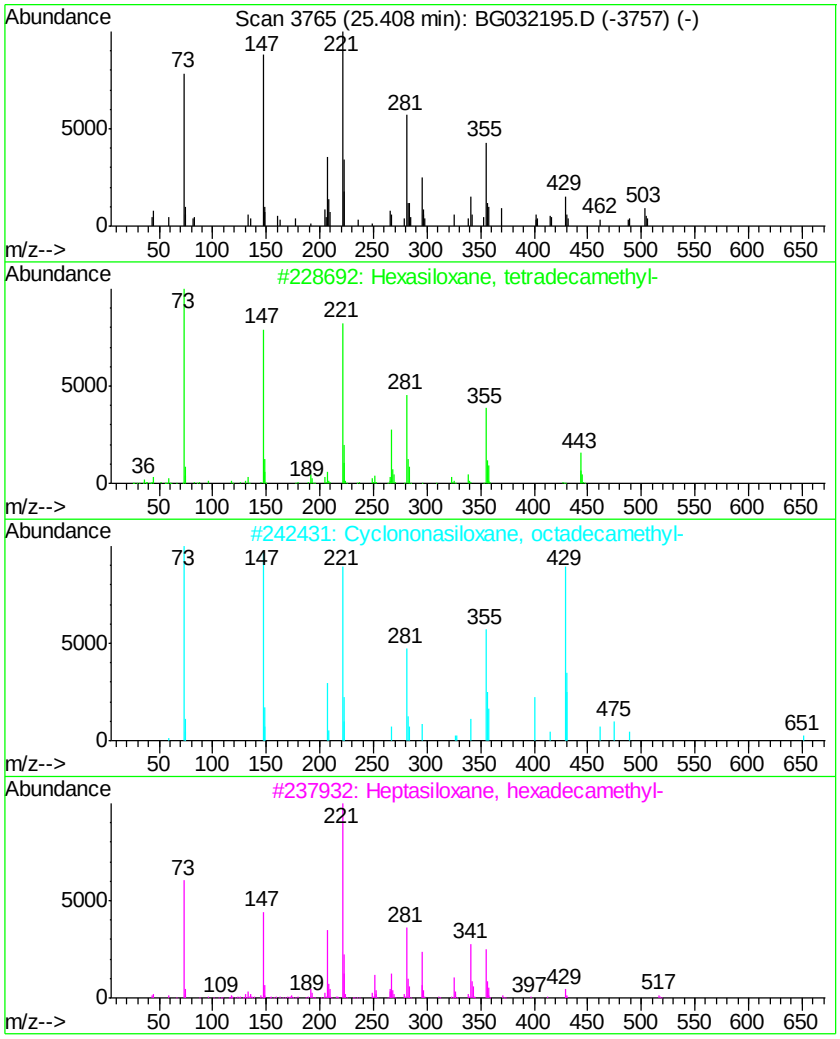
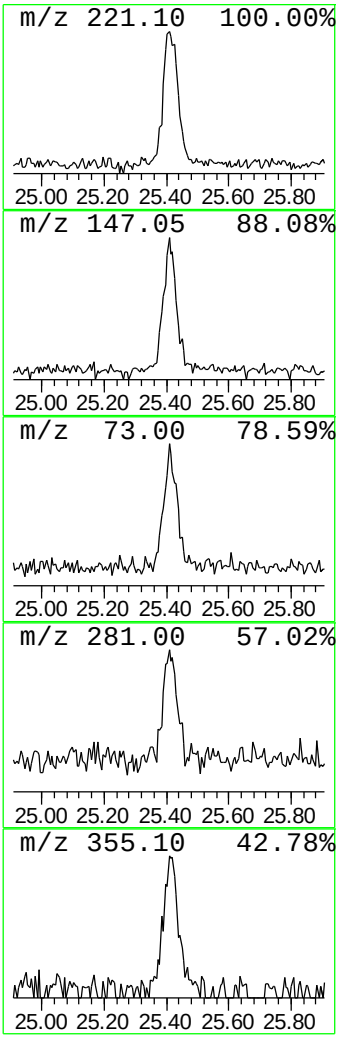
Peak Number 6 unknown25.41 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.41	2.02 ng	105717	Perylene-d12	26.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	45
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
4	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
5	Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22





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Sample : J1231-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BR-2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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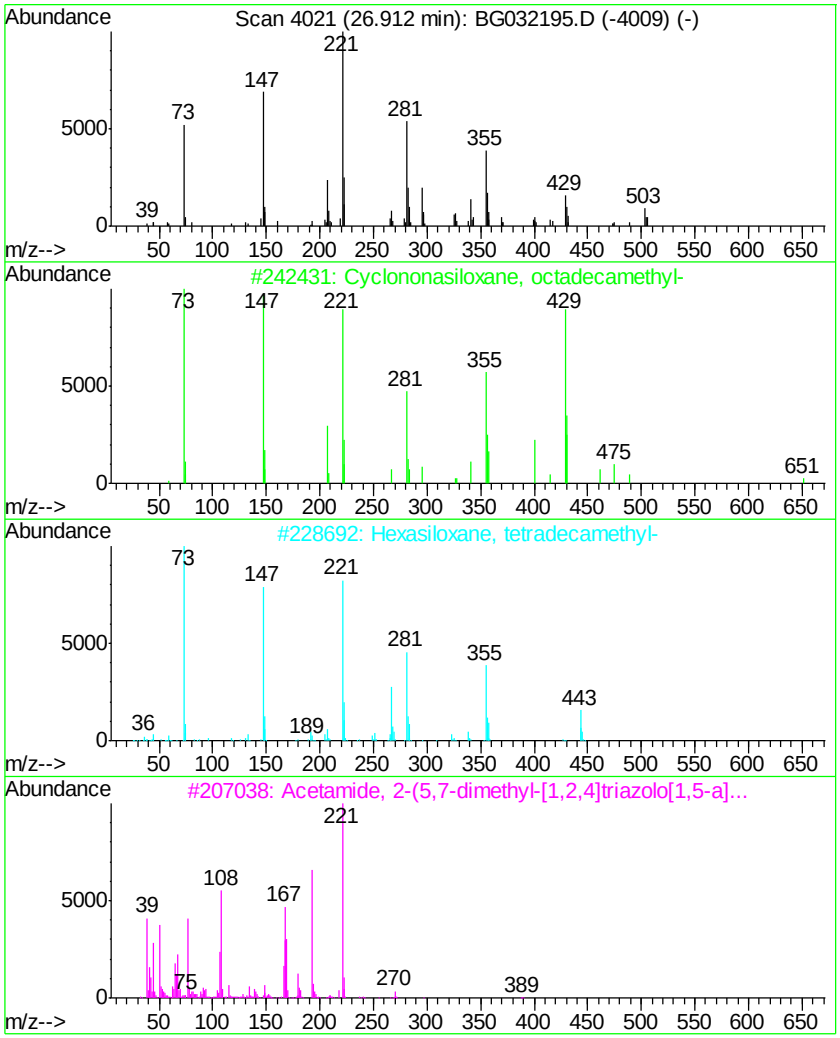
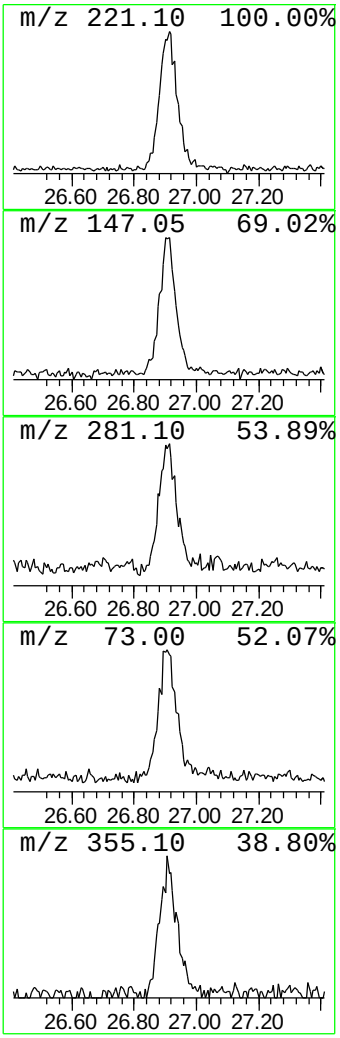
Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.91	4.76 ng	249813	Perylene-d12	26.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	74
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	37
3	Acetamide, 2-(5,7-dimethyl-[1,2,...	389	C21H19N5OS	1000304-63-9	30
4	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	27
5	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	22





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.67	4.3	ng	54509	1	8.74	255446	20.0
unknown8.26	8.26	95.8	ng	1224270	1	8.74	255446	20.0
Benzophenone	16.71	4.3	ng	112677	3	15.38	526497	20.0
5-Eicosene, (E)-	21.98	2.3	ng	116425	5	22.45	1022870	20.0
unknown25.41	25.41	2.0	ng	105717	6	26.14	1049100	20.0
Cyclononasiloxane...	26.91	4.8	ng	249813	6	26.14	1049100	20.0