LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
Data File : BG036956.D
Acq On : 25 Sep 2018 19:36
Operator : JU/SJ
Sample : J5061-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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	3.953	108	113	122	rBV	112138	178832	2.76%	0.812%
2	4.564	209	217	235	rBV	3700477	6472901	100.00%	29.388%
3	5.157	310	318	332	rBV	1012231	1687162	26.07%	7.660%
4	5.621	390	397	406	rBV	242425	454507	7.02%	2.064%
5	7.202	659	666	681	rBV	469040	952225	14.71%	4.323%
6	7.578	722	730	749	rBV	354003	708104	10.94%	3.215%
7	8.042	803	809	821	rBV	154793	293801	4.54%	1.334%
8	8.365	856	864	883	rBV	579755	1096489	16.94%	4.978%
9	8.688	912	919	933	rBV	103274	208883	3.23%	0.948%
10	9.205	999	1007	1019	rBV	442030	916450	14.16%	4.161%
11	10.845	1279	1286	1307	rBV	205377	413900	6.39%	1.879%
12	13.289	1695	1702	1717	rBV	1316449	2188118	33.80%	9.934%
13	14.670	1930	1937	1950	rBV2	342047	594757	9.19%	2.700%
14	16.156	2181	2190	2203	rBV2	101684	199792	3.09%	0.907%
15	17.413	2397	2404	2410	rBV	422049	723255	11.17%	3.284%
16	20.022	2842	2848	2859	rBV	2276752	3080182	47.59%	13.984%
17	21.679	3123	3130	3139	rBV	481663	837966	12.95%	3.804%
18	23.348	3408	3414	3426	rVB2	59824	115664	1.79%	0.525%
19	24.887	3666	3676	3690	rVB2	278060	835332	12.91%	3.793%
20	27.314	4081	4089	4090	rBV7	35844	67435	1.04%	0.306%

Sum of corrected areas: 22025755

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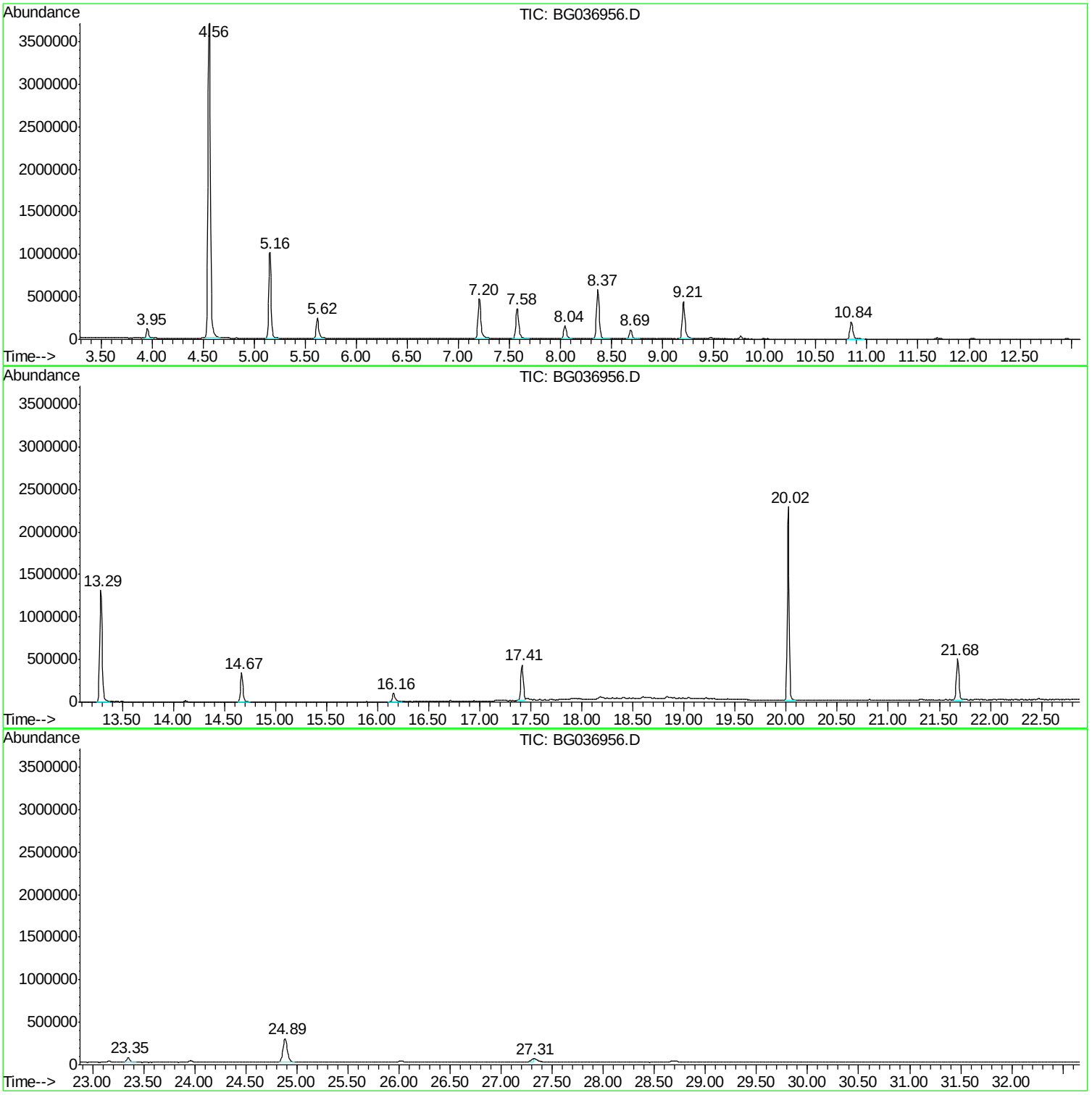
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092518\
Data File : BG036956.D
Acq On : 25 Sep 2018 19:36
Operator : JU/SJ
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

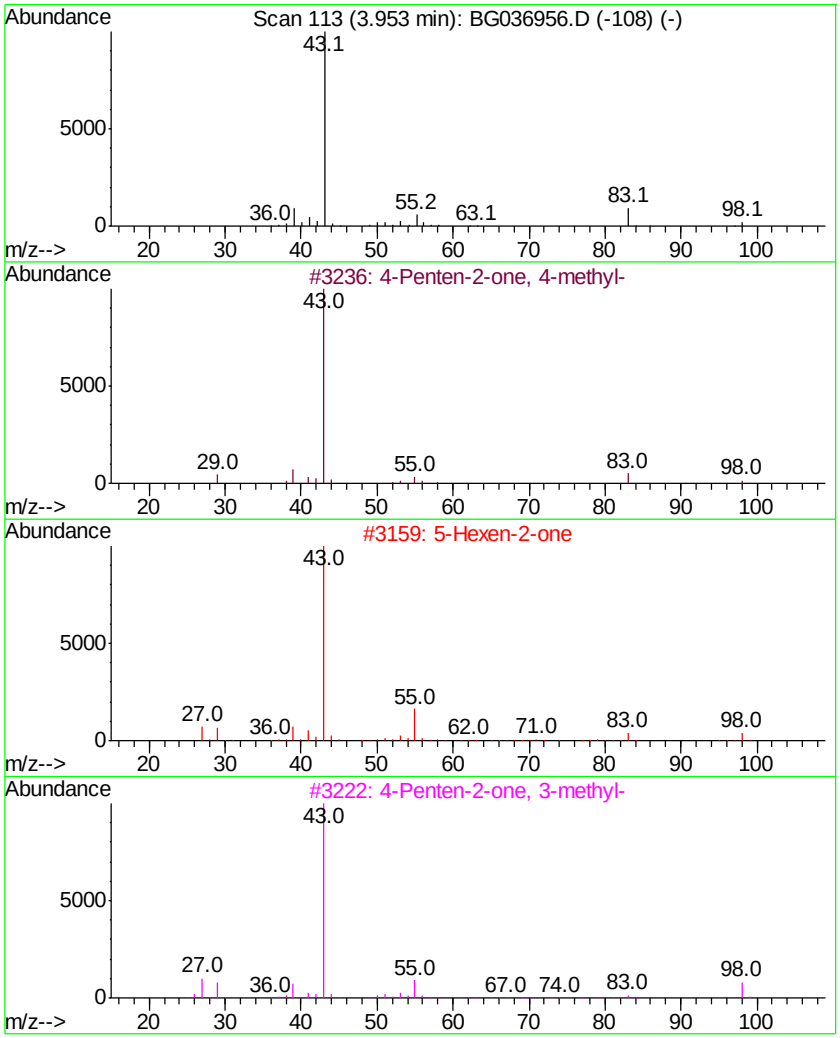
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

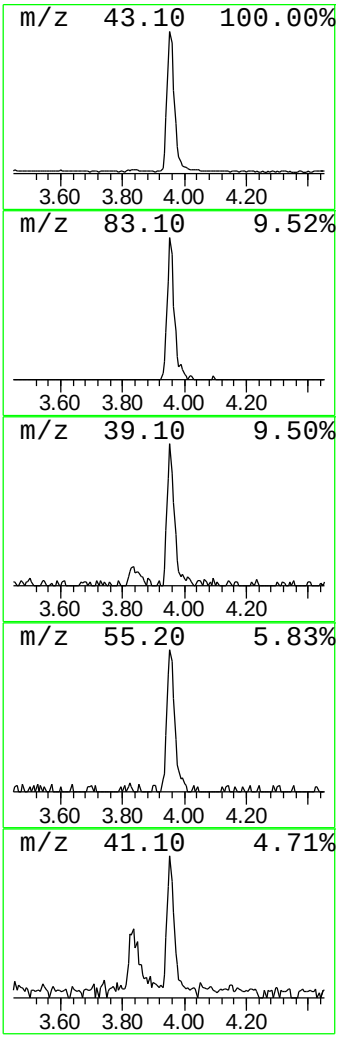
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	12.17 ng	178832	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	9





Library Search Compound Report

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Acq On : 25 Sep 2018 19:36
Operator : JU/SJ
Sample : J5061-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

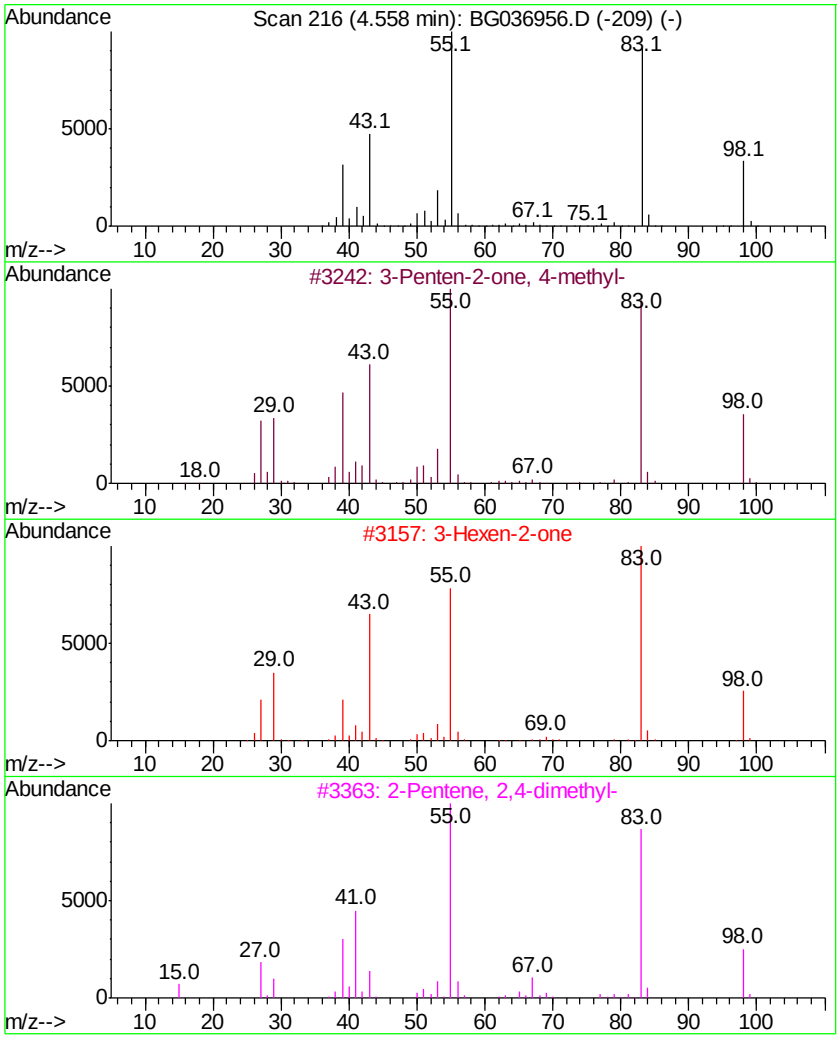
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

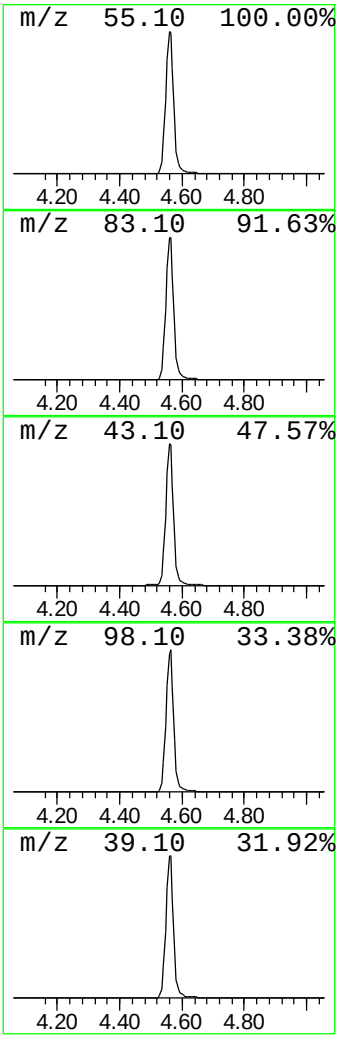
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	440.63 ng	6472900	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	78
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78





Library Search Compound Report

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Operator : JU/SJ
Sample : J5061-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

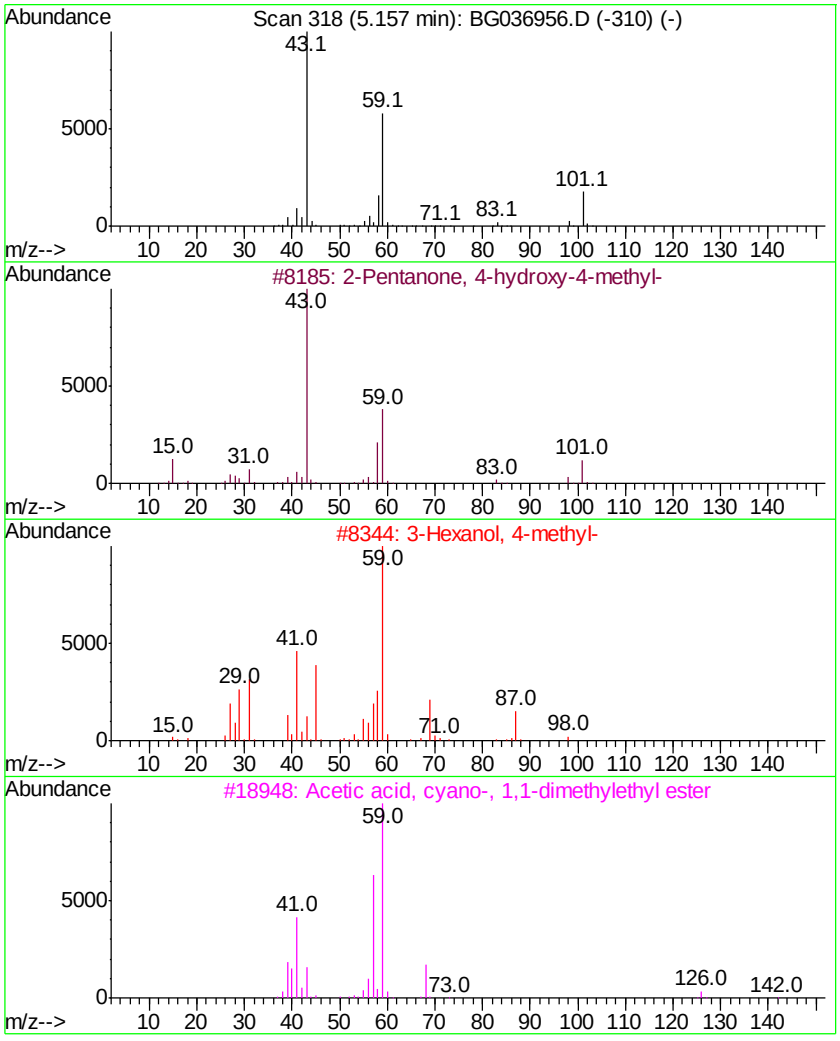
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

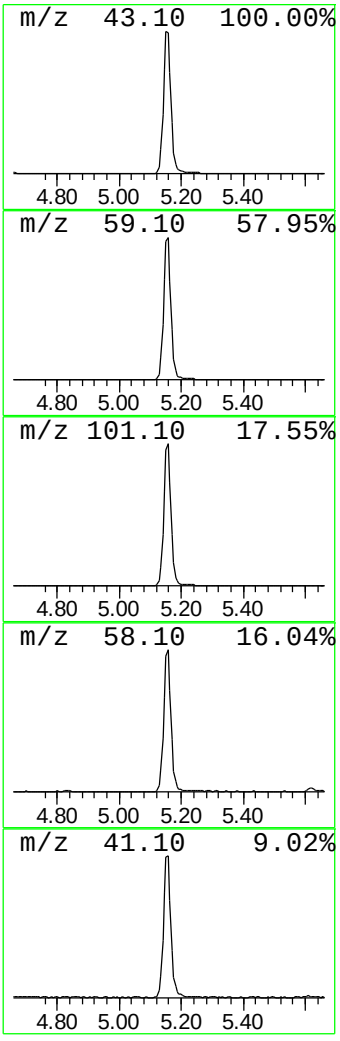
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	114.85 ng	1687160	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J5061-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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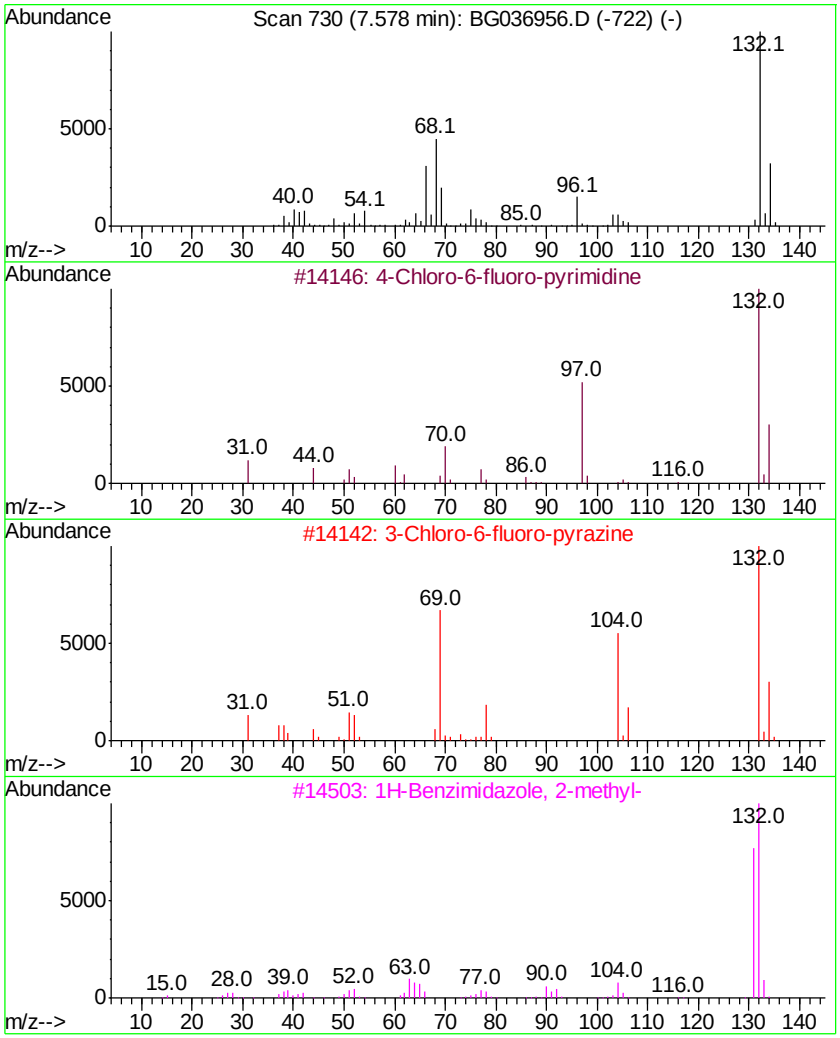
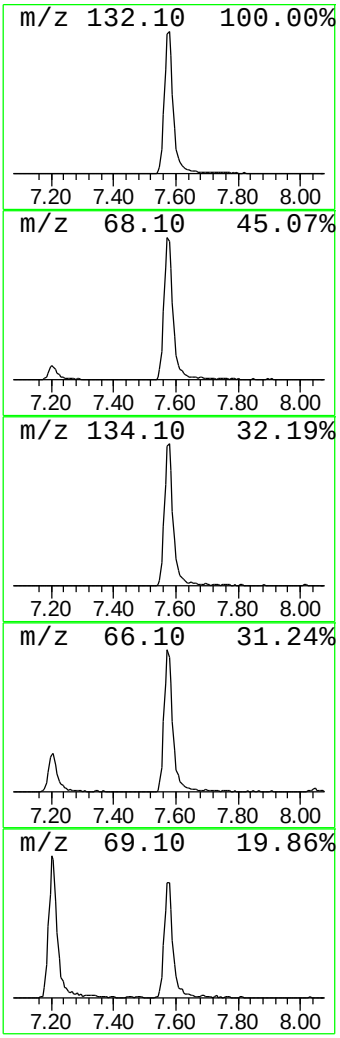
****

Peak Number 4 unknown7.58 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	48.20 ng	708104	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Operator : JU/SJ
Sample : J5061-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 230-KV-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

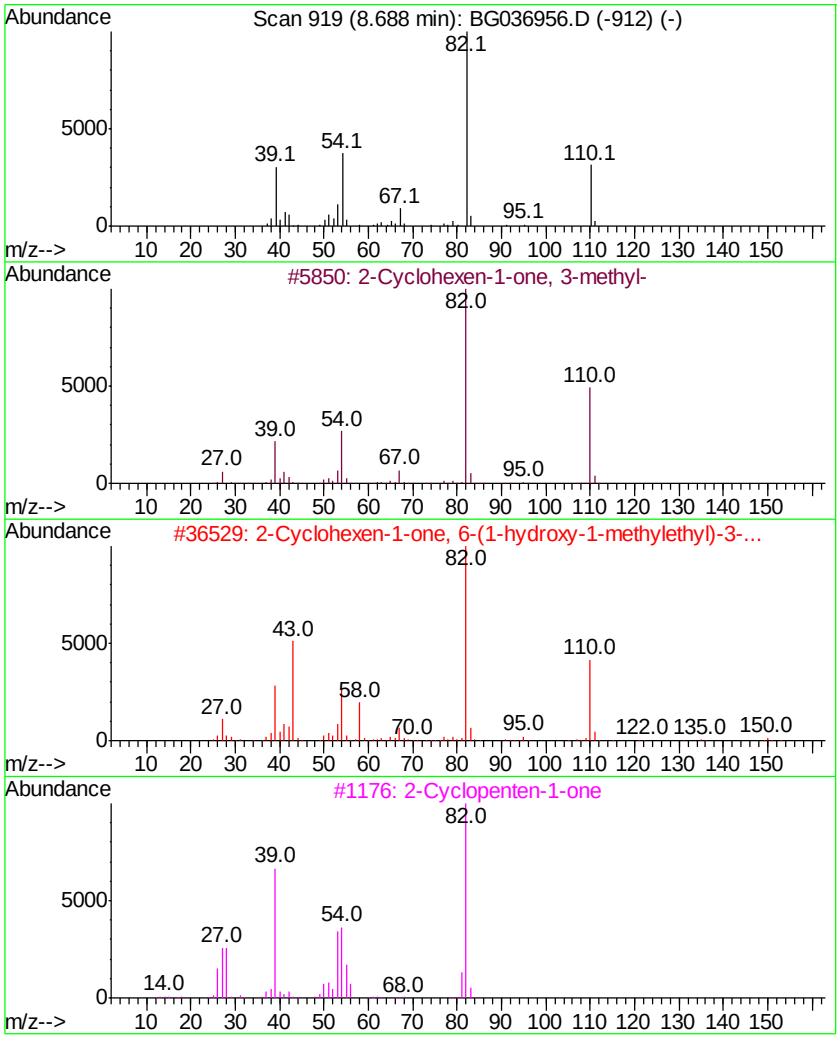
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

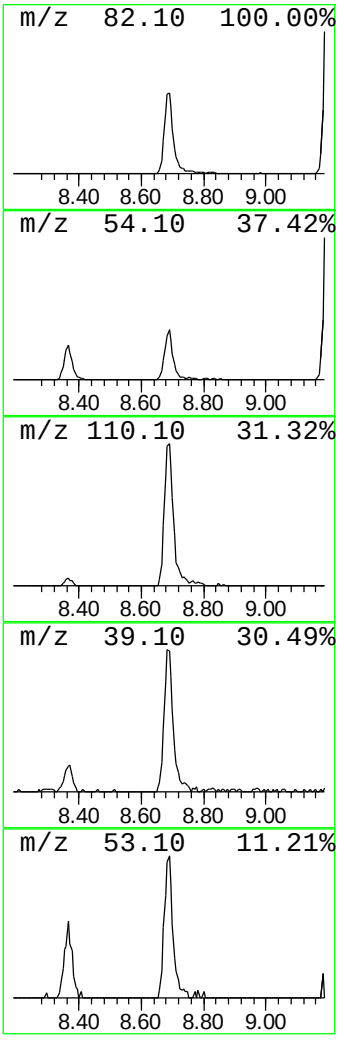
****

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	14.22 ng	208883	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	74
3	2-Cyclopenten-1-one	82	C5H6O	000930-30-3	50
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	45
5	1H-Imidazole, 4-methyl-	82	C4H6N2	000822-36-6	42





Library Search Compound Report

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TIC Library : C:\Database\NIST11.L
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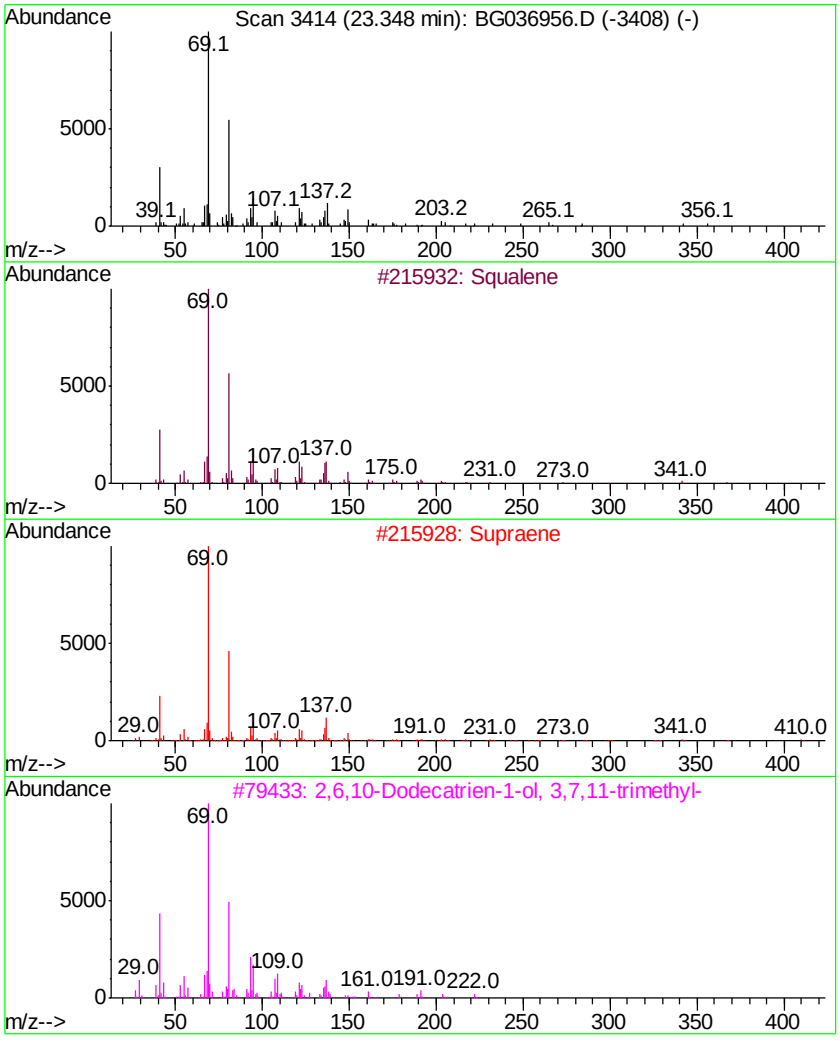
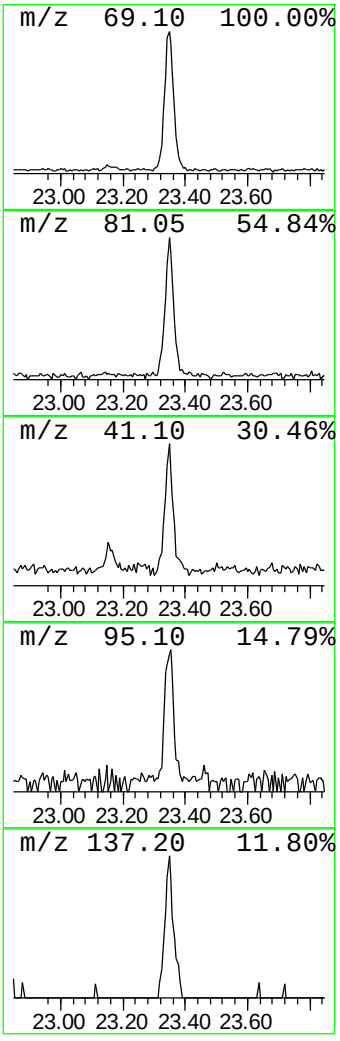
****

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.77 ng	115664	Perylene-d12	24.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80
4	Farnesol isomer a	222	C15H26O	1000108-92-4	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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
4-Penten-2-one, 4...	3.95	12.2	ng	178832	1	8.04	293801	20.0
3-Penten-2-one, 4...	4.56	440.6	ng	6472900	1	8.04	293801	20.0
2-Pentanone, 4-hy...	5.16	114.8	ng	1687160	1	8.04	293801	20.0
unknown7.58	7.58	48.2	ng	708104	1	8.04	293801	20.0
2-Cyclohexen-1-on...	8.69	14.2	ng	208883	1	8.04	293801	20.0
Squalene	23.35	2.8	ng	115664	6	24.88	835332	20.0