LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

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-BG083116.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	2.920	9	14	25	rVB	736924	1215318	92.94%	9.908%
2	4.500	281	283	287	rVB2	14545	16864	1.29%	0.137%
3	5.117	384	388	396	rVB	65515	110202	8.43%	0.898%
4	5.605	465	471	478	rBV2	112143	208661	15.96%	1.701%
5	7.009	706	710	716	rVB6	10060	18362	1.40%	0.150%
6	7.226	741	747	762	rVB	137382	280368	21.44%	2.286%
7	7.584	802	808	817	rBV2	141334	266028	20.34%	2.169%
8	8.048	880	887	893	rBV	270934	472146	36.11%	3.849%
9	8.372	934	942	949	rBV	132258	232190	17.76%	1.893%
10	9.229	1082	1088	1100	rBV	95739	202651	15.50%	1.652%
11	10.880	1362	1369	1380	rBV	395121	697175	53.32%	5.684%
12	13.335	1781	1787	1796	rBV	267378	431381	32.99%	3.517%
13	13.576	1824	1828	1831	rBV5	16441	23896	1.83%	0.195%
14	14.029	1898	1905	1913	rVB2	199612	302050	23.10%	2.462%
15	14.175	1925	1930	1936	rBV2	65249	110478	8.45%	0.901%
16	14.340	1952	1958	1964	rBV	393961	515301	39.41%	4.201%
17	14.416	1966	1971	1975	rBV3	40483	65528	5.01%	0.534%
18	14.493	1979	1984	1987	rVV2	86095	123761	9.46%	1.009%
19	14.522	1987	1989	1994	rVV3	32754	41381	3.16%	0.337%
20	14.569	1994	1997	2004	rVB7	8849	17480	1.34%	0.143%
21	14.640	2004	2009	2013	rBV2	29860	49930	3.82%	0.407%
22	14.681	2013	2016	2019	rVV3	80730	111141	8.50%	0.906%
23	14.722	2019	2023	2029	rVV2	548959	887334	67.86%	7.234%
24	14.786	2031	2034	2040	rVV8	25187	52036	3.98%	0.424%
25	14.857	2042	2046	2050	rVB3	30365	40784	3.12%	0.332%
26	14.957	2058	2063	2066	rBV5	30735	51025	3.90%	0.416%
27	14.992	2066	2069	2075	rVB3	61455	87655	6.70%	0.715%
28	15.386	2130	2136	2142	rBV2	134664	190127	14.54%	1.550%
29	15.679	2180	2186	2189	rBV4	19853	30442	2.33%	0.248%
30	15.726	2189	2194	2199	rVB4	41965	71771	5.49%	0.585%
31	15.838	2210	2213	2219	rVB8	12705	19333	1.48%	0.158%
32	16.155	2264	2267	2272	rBV5	20625	36018	2.75%	0.294%
33	16.231	2273	2280	2289	rVB5	78430	213475	16.33%	1.740%
34	16.402	2304	2309	2310	rBV5	11910	17875	1.37%	0.146%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

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-BG083116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.455	2316	2318	2325	rVB8	17279	25680	1.96%	0.209%
36	16.566	2333	2337	2338	rBV4	12011	14720	1.13%	0.120%
37	16.731	2360	2365	2366	rBV5	9351	13239	1.01%	0.108%
38	16.837	2378	2383	2391	rVB3	154260	246312	18.84%	2.008%
39	16.936	2396	2400	2406	rVV6	43676	62086	4.75%	0.506%
40	17.001	2408	2411	2415	rVB6	12629	16696	1.28%	0.136%
41	17.489	2488	2494	2503	rBV	610315	989519	75.67%	8.067%
42	18.223	2613	2619	2628	rVB	970995	1307608	100.00%	10.660%
43	18.311	2630	2634	2635	rBV4	20967	25097	1.92%	0.205%
44	18.370	2639	2644	2647	rBV6	19940	31713	2.43%	0.259%
45	19.057	2758	2761	2768	rBV9	21069	49535	3.79%	0.404%
46	19.774	2879	2883	2887	rBV4	47160	57538	4.40%	0.469%
47	20.097	2934	2938	2943	rBV	397252	521462	39.88%	4.251%
48	21.800	3223	3228	3235	rVB	619694	993480	75.98%	8.099%
49	25.149	3794	3798	3810	rVB	243067	701673	53.66%	5.720%

Sum of corrected areas: 12266525

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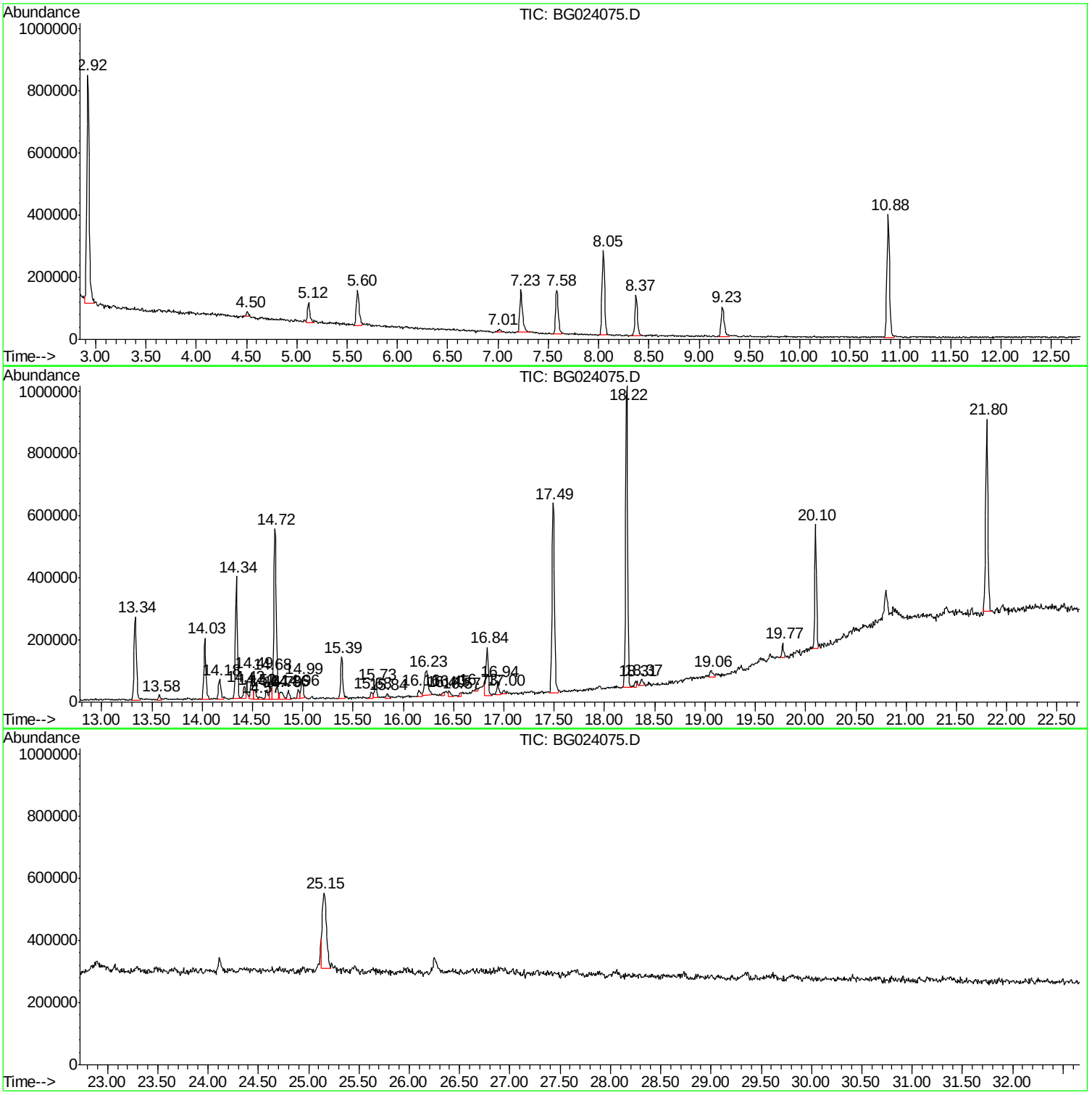
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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\BG092216\
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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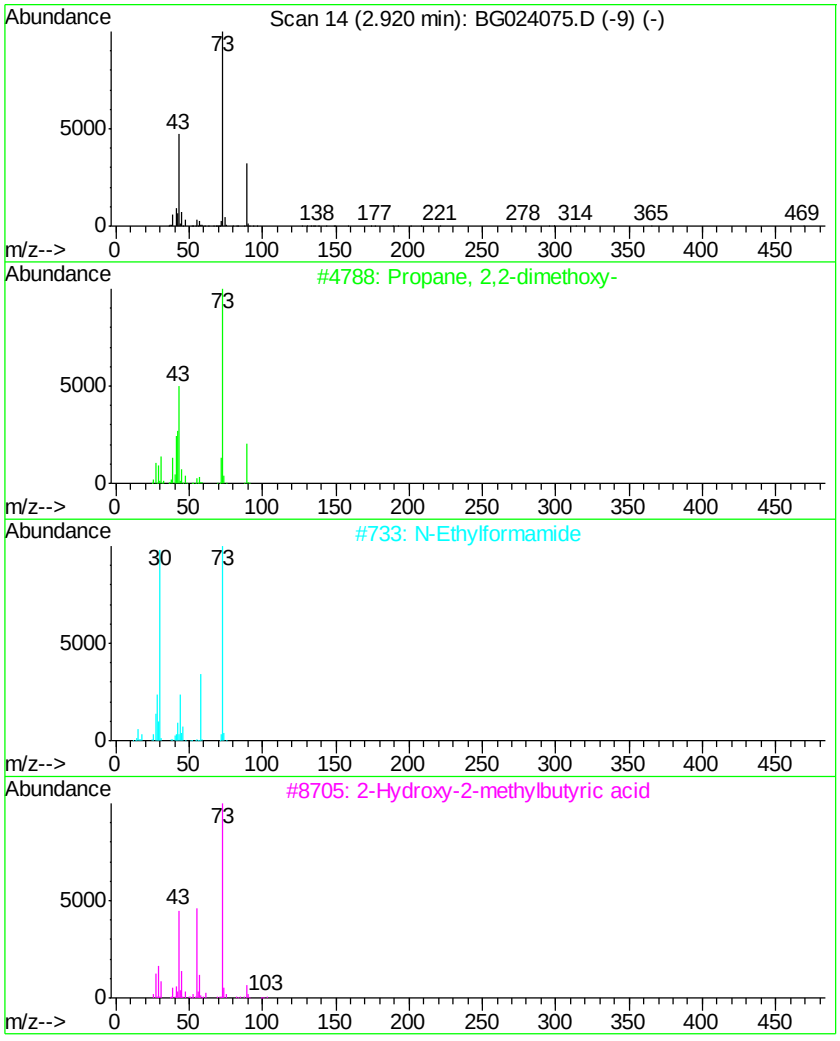
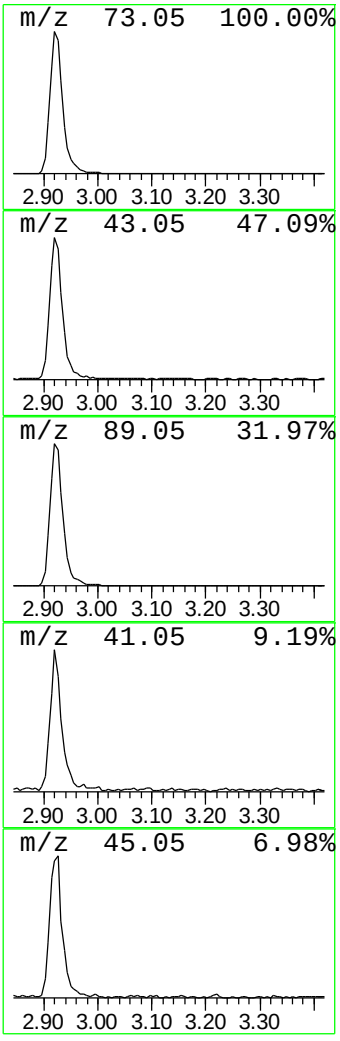
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	51.48 ng	1215320	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
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Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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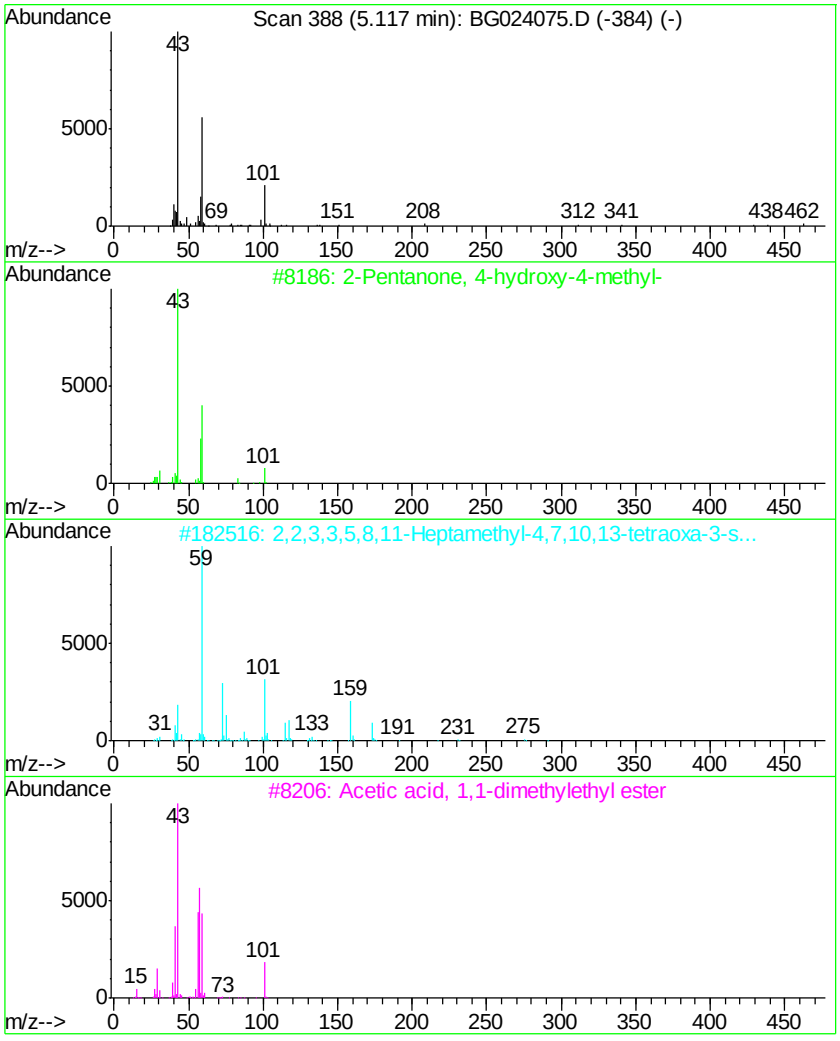
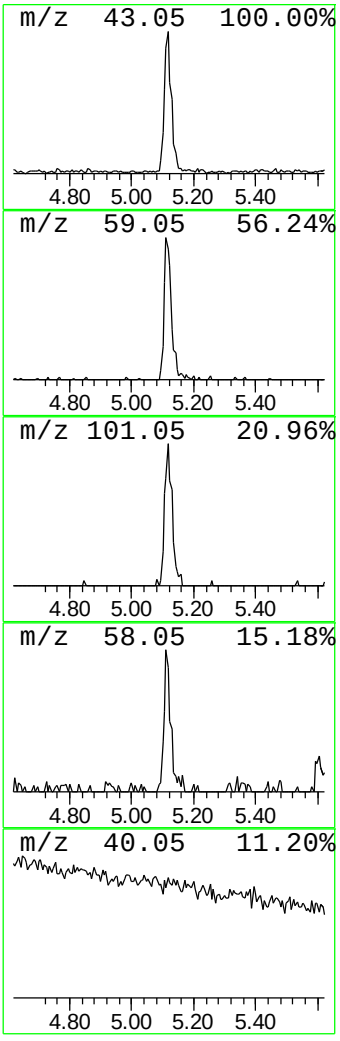
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.67 ng	110202	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,2,3,3,5,8,11-Heptamethyl-4,7,1...	348	C18H40O4Si	1000367-07-2	43
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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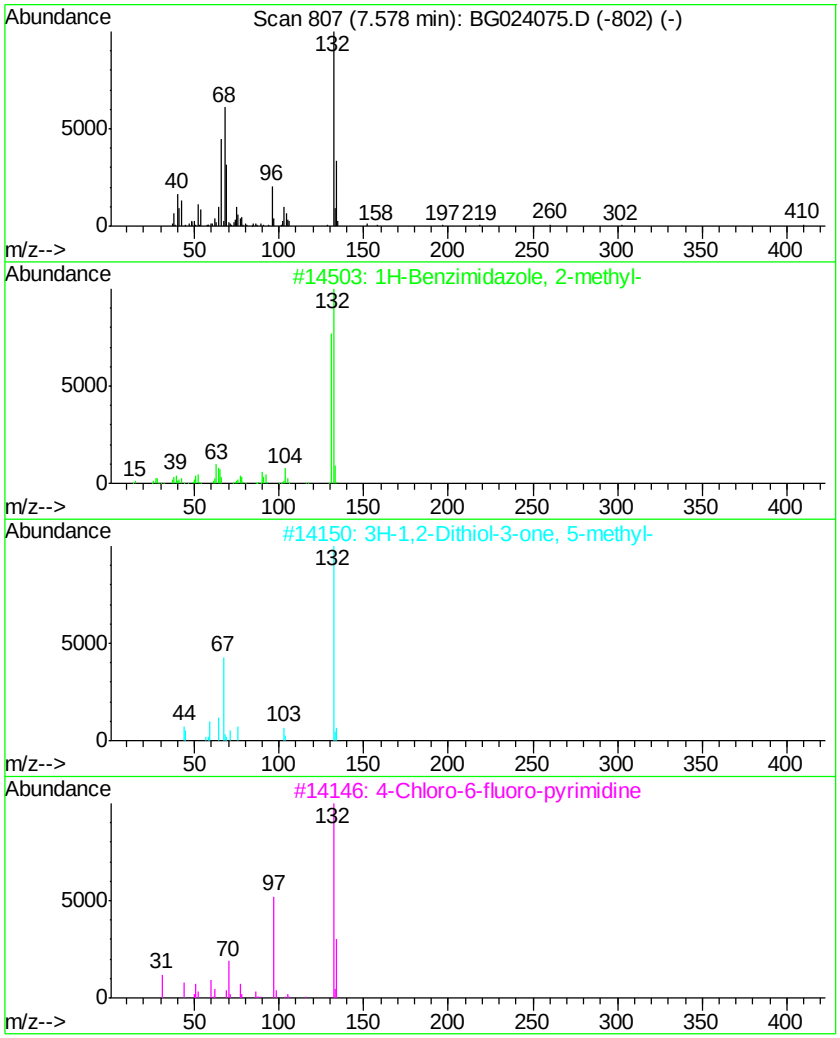
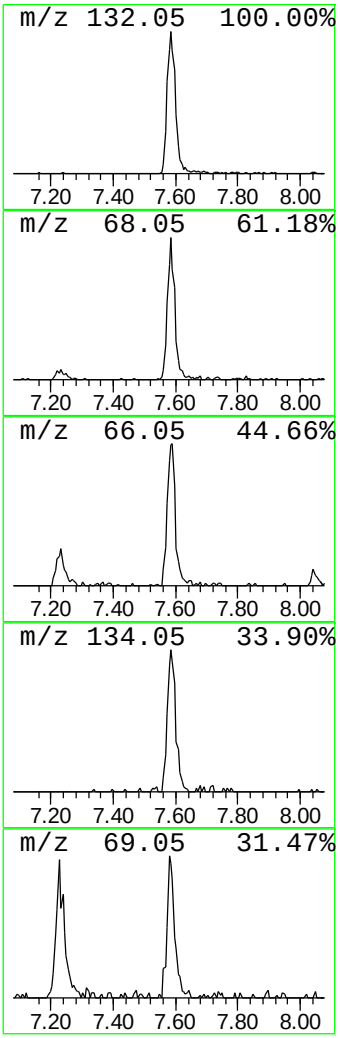
Peak Number 3 unknown7.58 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	11.27 ng	266028	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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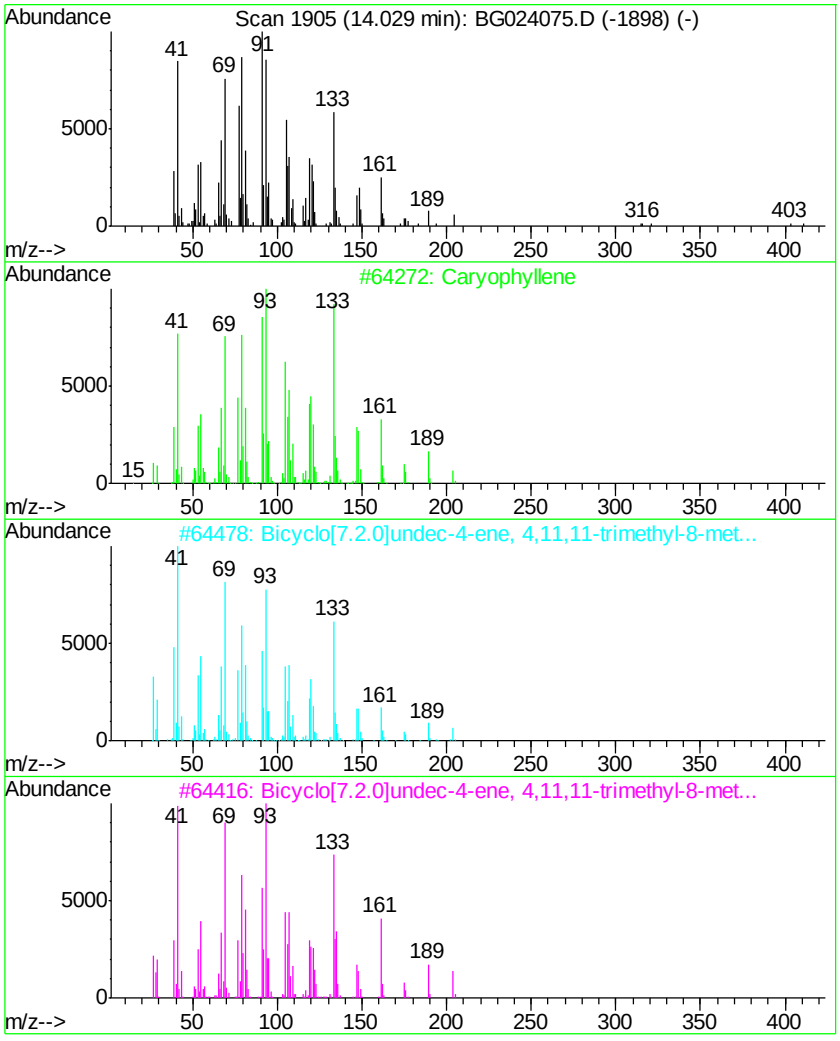
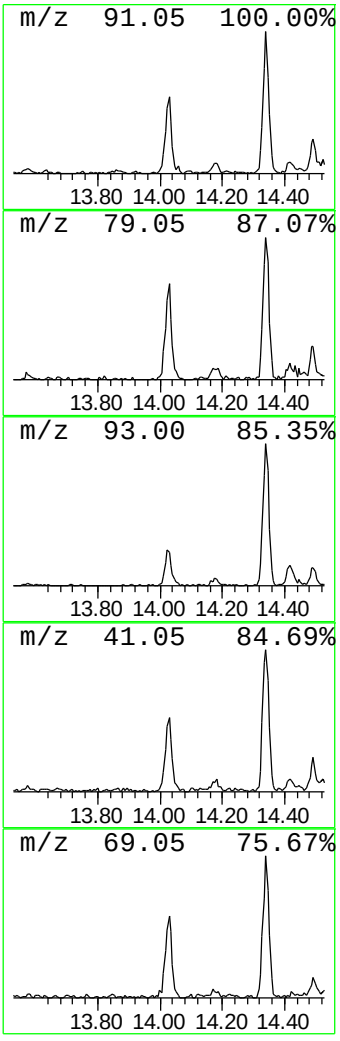
Peak Number 5 Caryophyllene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	6.81 ng	302050	Acenaphthene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	96
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	90
4	Isocaryophillene	204	C15H24	1000140-07-2	70
5	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	41





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Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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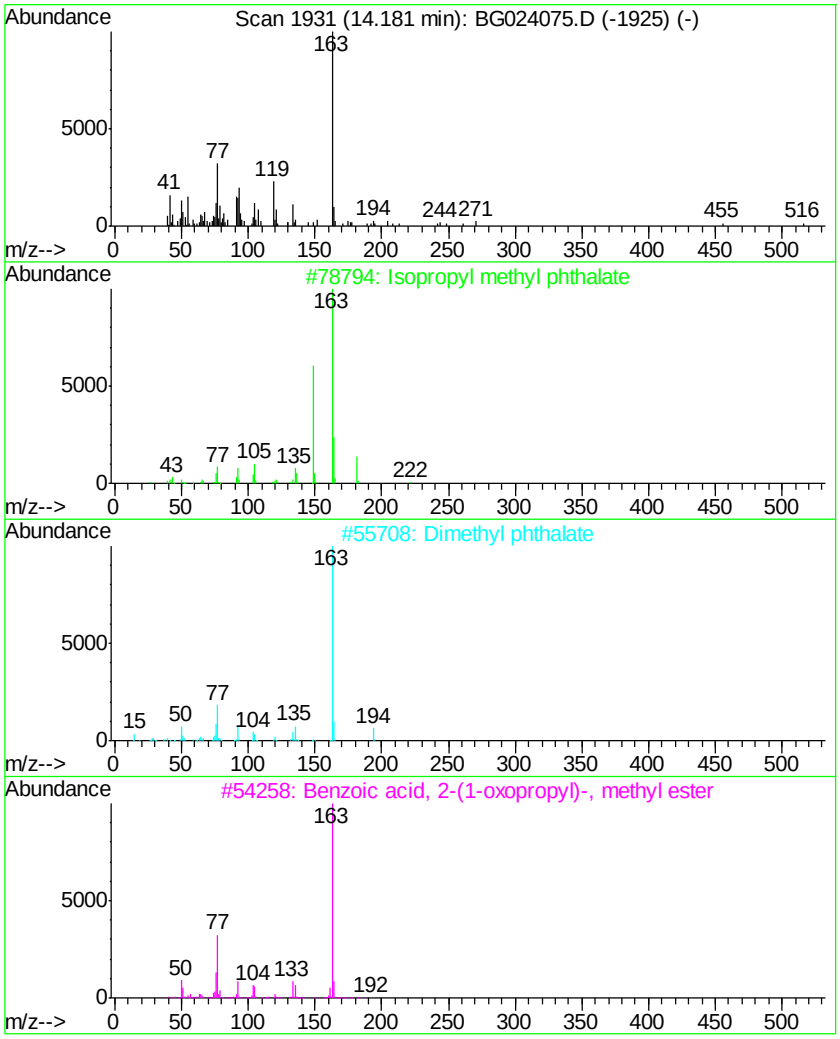
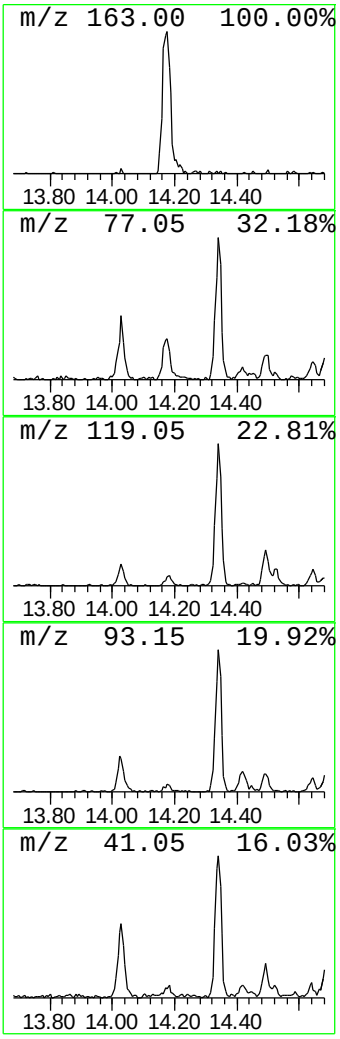
Peak Number 6 Isopropyl methyl phthalate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	2.49 ng	110478	Acenaphthene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl methyl phthalate	222	C12H14O4	071369-19-2	53
2	Dimethyl phthalate	194	C10H10O4	000131-11-3	53
3	Benzoic acid, 2-(1-oxopropyl)-, ...	192	C11H12O3	032025-37-9	53
4	p-Amidinobenzamide	163	C8H9N3O	054050-86-1	47
5	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	43





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Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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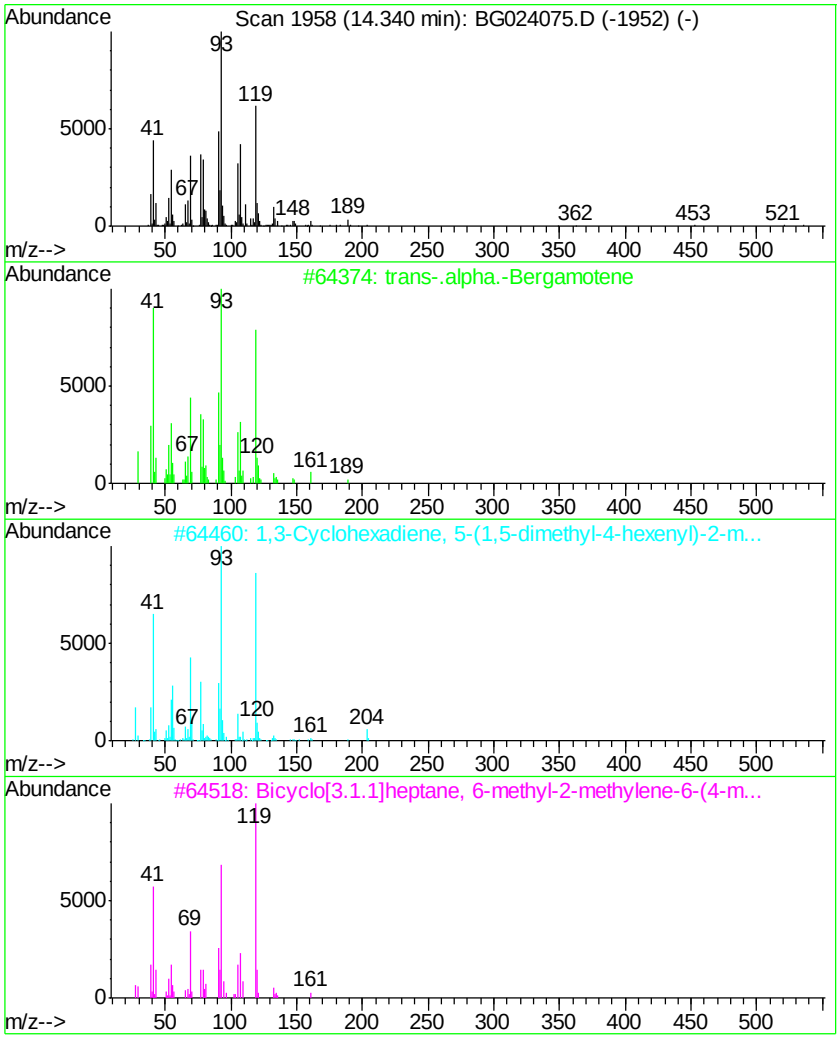
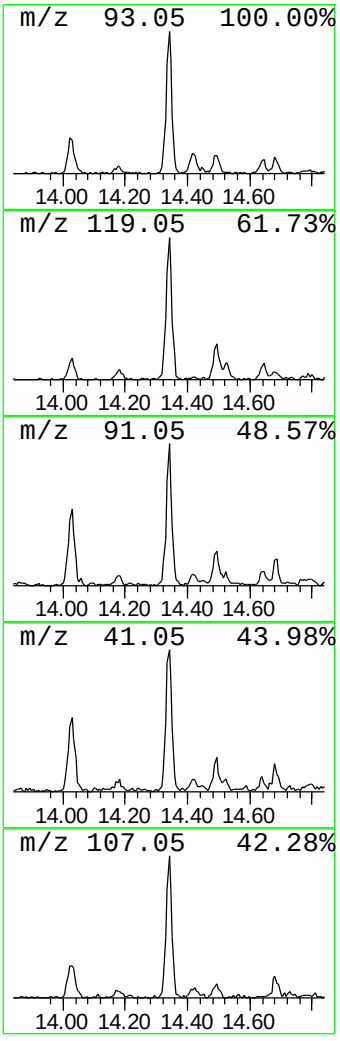
Peak Number 7 trans-.alpha.-Bergamotene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	11.61 ng	515301	Acenaphthene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	64
2	1,3-Cyclohexadiene, 5-(1,5-dimet...	204	C15H24	000495-60-3	50
3	Bicyclo[3.1.1]heptane, 6-methyl-...	204	C15H24	055123-21-2	50
4	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	41
5	3-(2-Pyridyl)propyl trifluoroace...	233	C10H10F3NO2	1000373-16-8	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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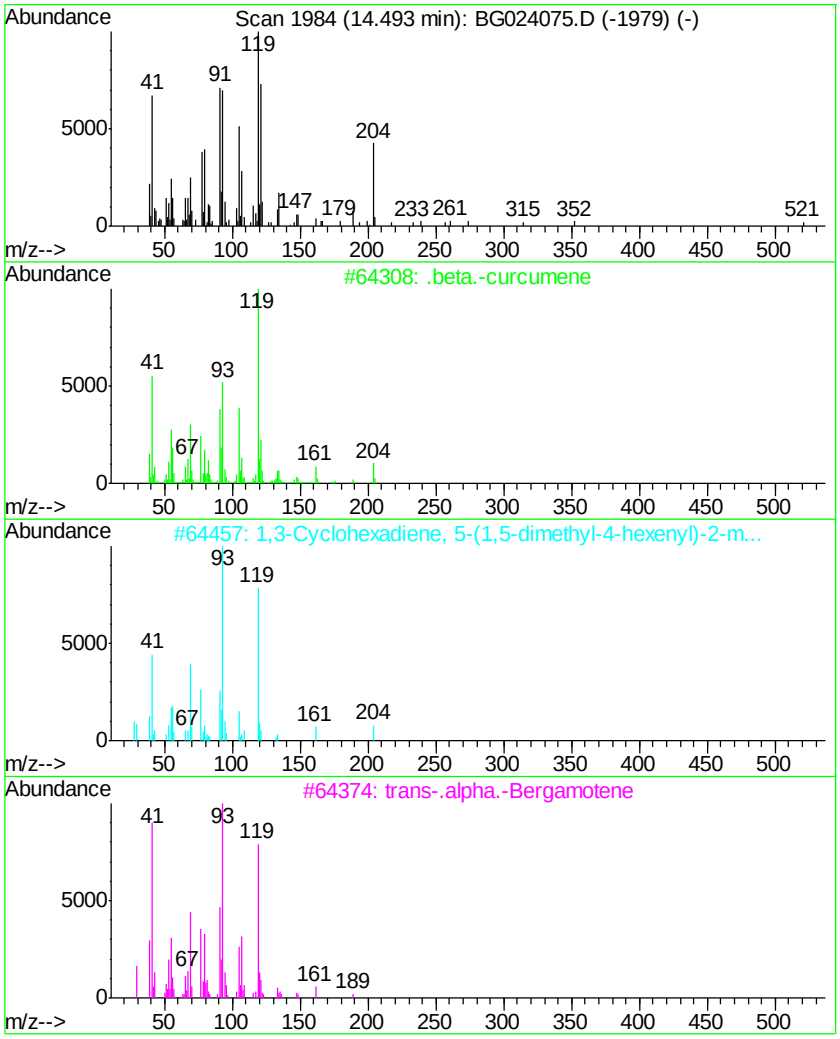
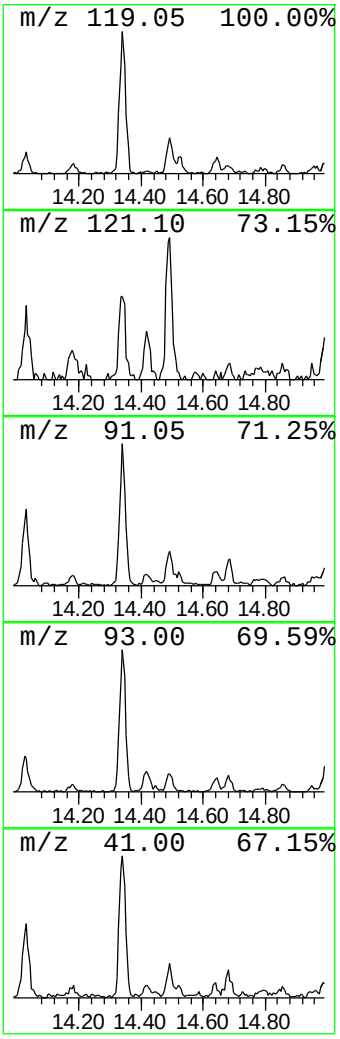
Peak Number 8 .beta.-curcumene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.79 ng	123761	Acenaphthene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-curcumene	204	C15H24	1000374-17-4	60
2	1,3-Cyclohexadiene, 5-(1,5-dimet...	204	C15H24	000495-60-3	38
3	trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	27
4	2H-1,2,4-Triazol-3-amine, N-(4-m...	204	C10H12N4O	103038-24-0	25
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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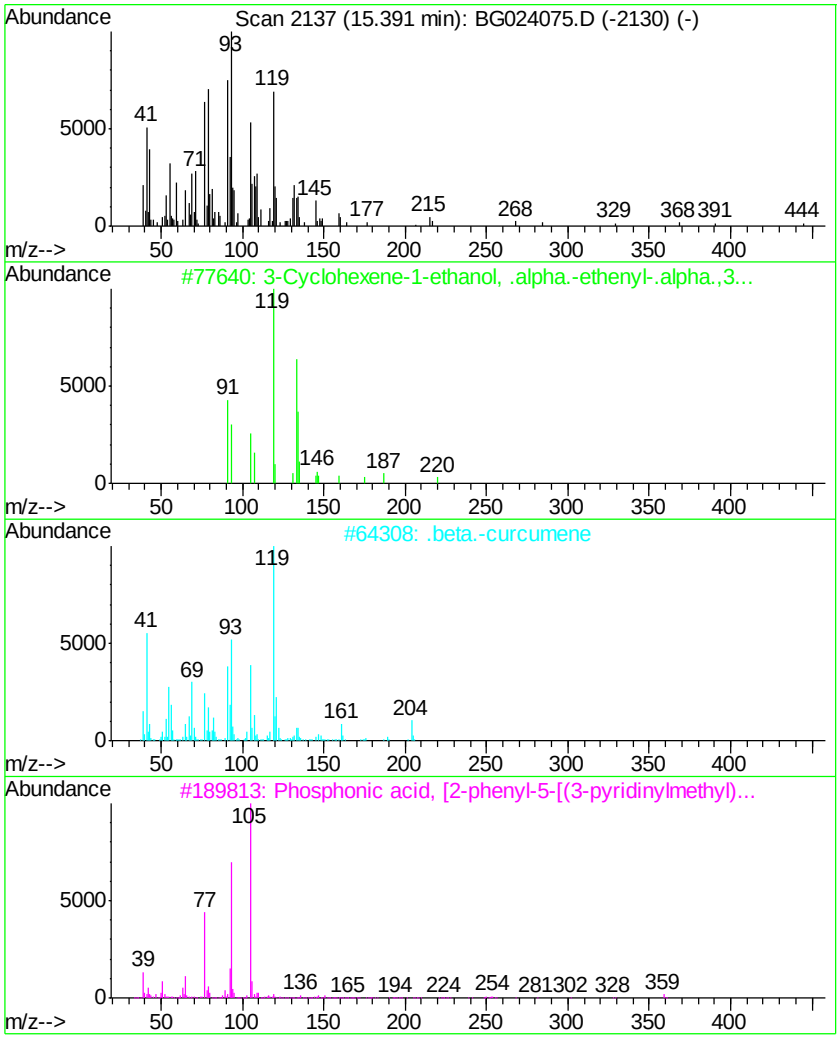
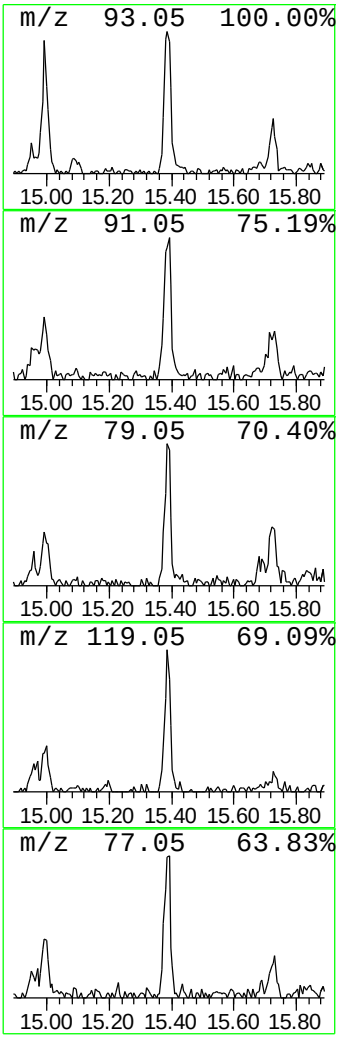
Peak Number 9 unknown15.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	4.29 ng	190127	Acenaphthene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-ethanol, .alpha....	220	C15H24O	055780-93-3	43
2	.beta.-curcumene	204	C15H24	1000374-17-4	35
3	Phosphonic acid, [2-phenyl-5-[(3...	359	C17H18N3O4P	1000349-98-1	35
4	trans-.beta.-Ocimene	136	C10H16	003779-61-1	27
5	6-(p-Tolyl)-2-methyl-2-heptenol,...	218	C15H22O	039599-18-3	27





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Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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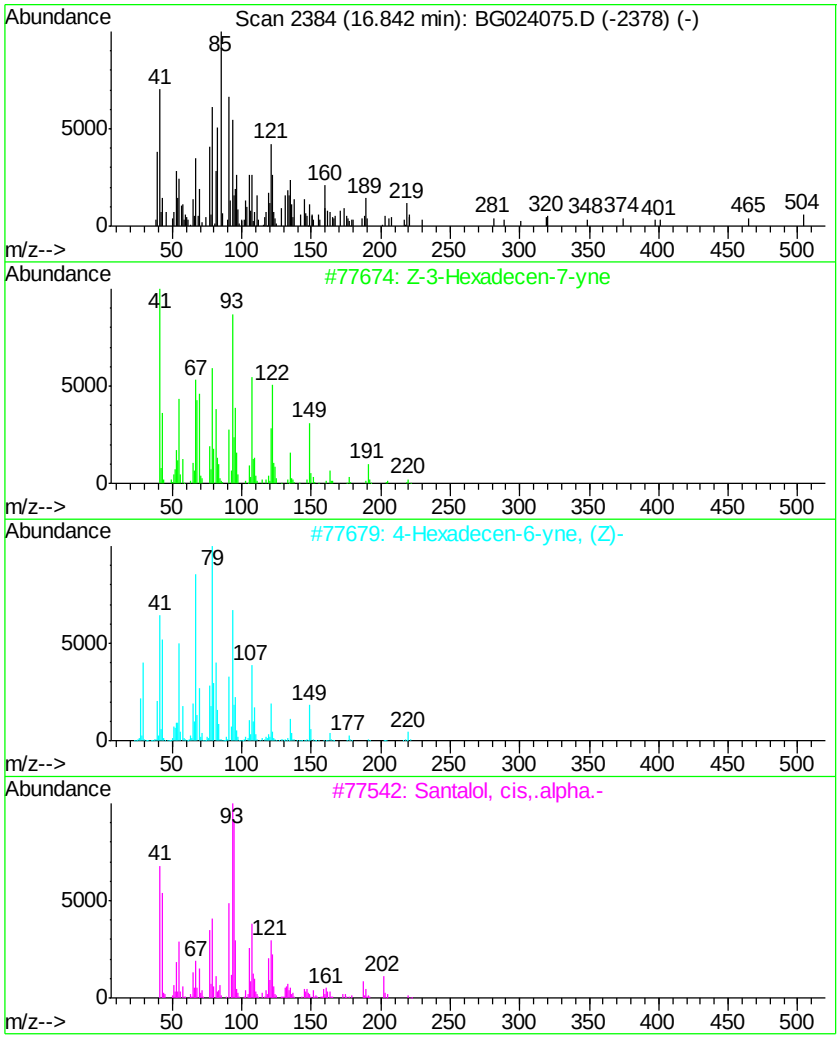
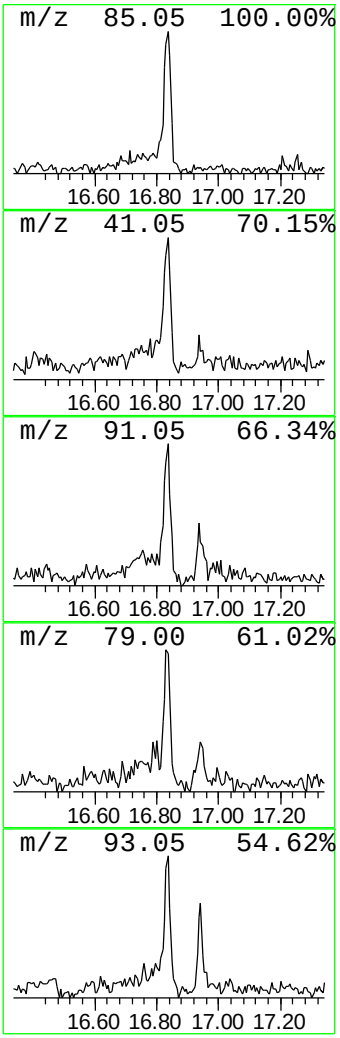
Peak Number 10 Z-3-Hexadecen-7-yne Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	4.98 ng	246312	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-3-Hexadecen-7-yne	220	C16H28	1000130-91-3	58
2	4-Hexadecen-6-yne, (Z)-	220	C16H28	074744-54-0	43
3	Santalol, cis,.alpha.-	220	C15H24O	019903-72-1	35
4	1,5-Cyclooctadiene, 3-(1-methyl-...	162	C12H18	016538-88-8	30
5	Caryophyllene oxide	220	C15H24O	001139-30-6	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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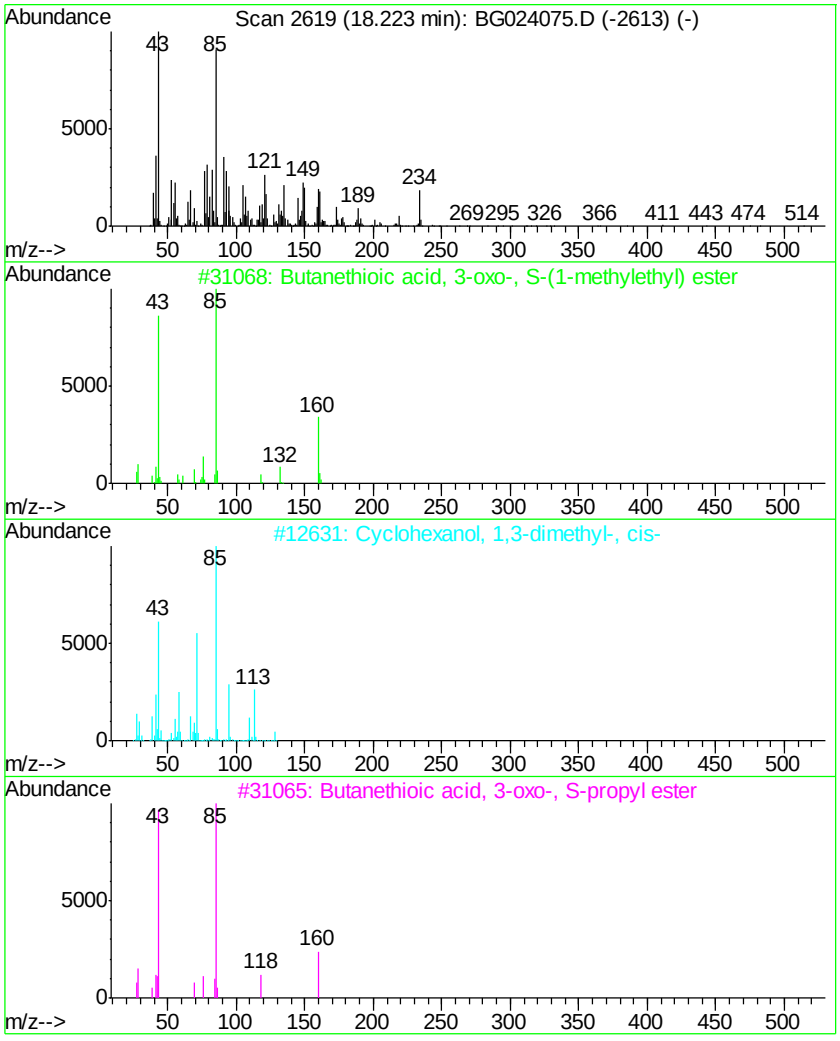
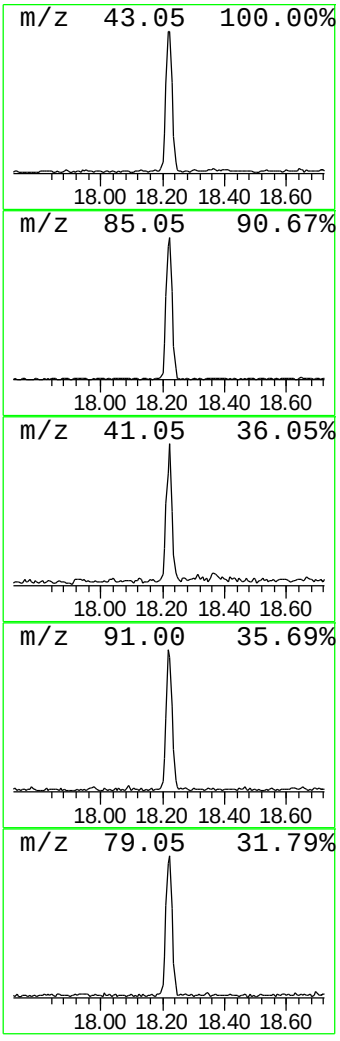
Peak Number 11 unknown18.22 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	26.43 ng	1307610	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanethioic acid, 3-oxo-, S-(1-...	160	C7H12O2S	015780-62-8	35
2	Cyclohexanol, 1,3-dimethyl-, cis-	128	C8H16O	015466-94-1	35
3	Butanethioic acid, 3-oxo-, S-pro...	160	C7H12O2S	015780-61-7	35
4	10-Methylundecan-4-olide	198	C12H22O2	1000370-40-5	30
5	2H-Pyran-2-methanol, tetrahydro-	116	C6H12O2	000100-72-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092216\
Data File : BG024075.D
Acq On : 22 Sep 2016 19:05
Operator : UM/SJ
Sample : H4821-13 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : YORK-SB1-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
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
Propane, 2,2-dime...	2.92	51.5	ng	1215320	1	8.05	472146	20.0
2-Pentanone, 4-hy...	5.12	4.7	ng	110202	1	8.05	472146	20.0
unknown7.58	7.58	11.3	ng	266028	1	8.05	472146	20.0
Caryophyllene	14.03	6.8	ng	302050	3	14.72	887334	20.0
Isopropyl methyl ...	14.18	2.5	ng	110478	3	14.72	887334	20.0
trans-.alpha.-Ber...	14.34	11.6	ng	515301	3	14.72	887334	20.0
.beta.-curcumene	14.49	2.8	ng	123761	3	14.72	887334	20.0
unknown15.39	15.39	4.3	ng	190127	3	14.72	887334	20.0
Z-3-Hexadecen-7-yne	16.84	5.0	ng	246312	4	17.49	989519	20.0
unknown18.22	18.22	26.4	ng	1307610	4	17.49	989519	20.0