LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024603.D
Acq On : 1 Nov 2016 21:44
Operator : UM/SJ
Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

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-BG102516.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	2.979	18	24	44	rVB	6346019	20258933	100.00%	19.074%
2	3.126	44	49	67	rVB	4616980	8729659	43.09%	8.219%
3	3.273	67	74	101	rVB	5141744	13830689	68.27%	13.022%
4	3.537	114	119	127	rBV2	125794	257498	1.27%	0.242%
5	5.329	418	424	432	rBV	660704	1081079	5.34%	1.018%
6	5.799	495	504	515	rBV	2873297	4857455	23.98%	4.573%
7	7.403	768	777	786	rBV	2976601	5391674	26.61%	5.076%
8	7.797	836	844	857	rVB	2817352	5107233	25.21%	4.808%
9	8.267	916	924	930	rBV	464107	812655	4.01%	0.765%
10	8.596	969	980	990	rBV	2132087	3864722	19.08%	3.639%
11	9.442	1116	1124	1134	rBV	1845301	3389677	16.73%	3.191%
12	11.093	1396	1405	1414	rBV	586305	1106055	5.46%	1.041%
13	13.508	1807	1816	1824	rBV	4627711	7411390	36.58%	6.978%
14	14.318	1946	1954	1961	rBV	1027757	1540588	7.60%	1.450%
15	14.883	2043	2050	2057	rBV	998255	1568545	7.74%	1.477%
16	16.363	2296	2302	2314	rBV	4055757	6503245	32.10%	6.123%
17	17.626	2506	2517	2524	rBV	1243881	1988709	9.82%	1.872%
18	20.206	2950	2956	2964	rVB	8743896	12117642	59.81%	11.409%
19	21.498	3171	3176	3183	rBV4	145123	261439	1.29%	0.246%
20	21.915	3241	3247	3255	rVB	1588007	2793613	13.79%	2.630%
21	23.643	3534	3541	3550	rVB	249469	505585	2.50%	0.476%
22	25.347	3818	3831	3843	rVB3	931924	2835524	14.00%	2.670%

Sum of corrected areas: 106213609

LSC Report - Integrated Chromatogram

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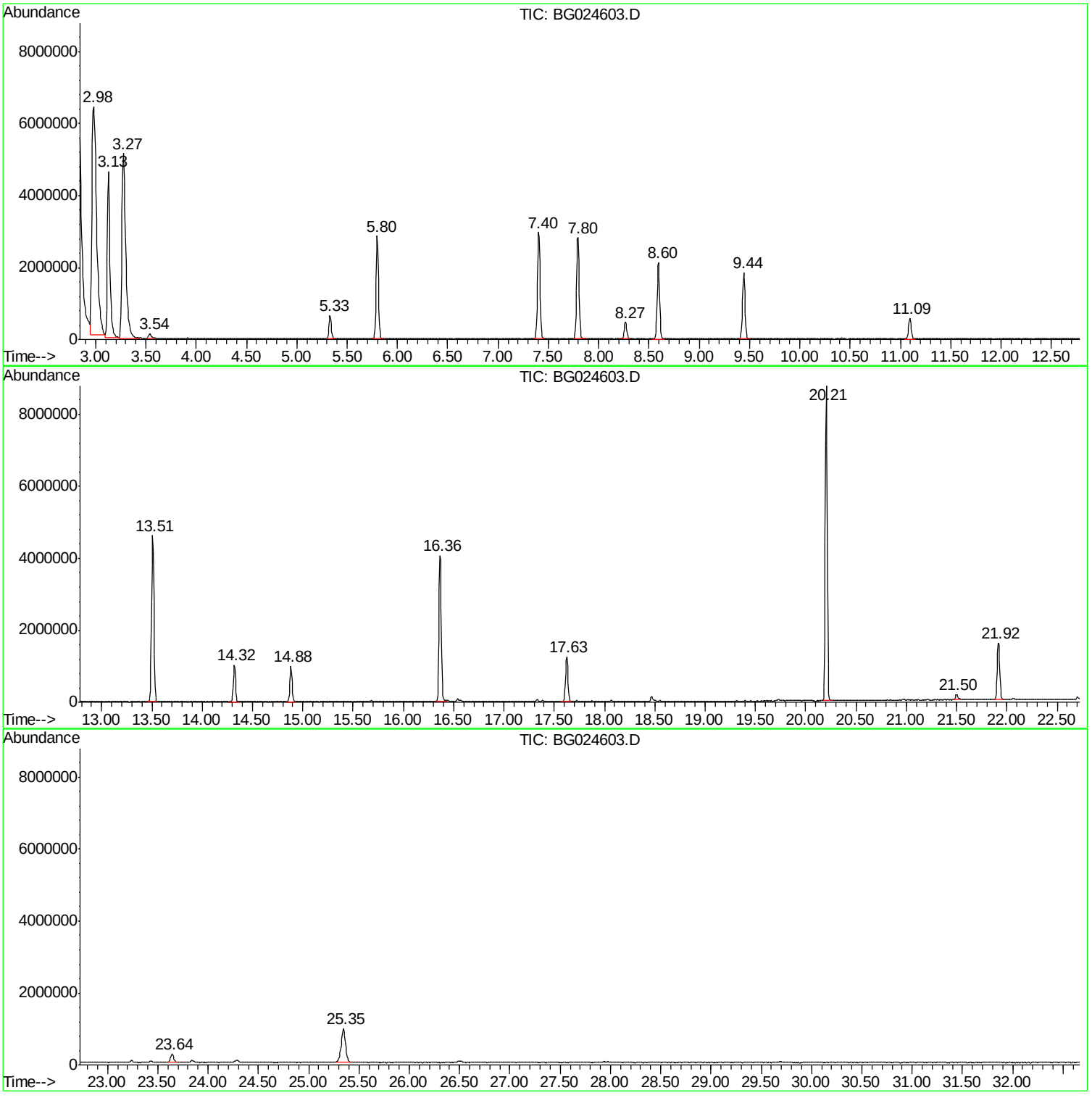
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024603.D
Acq On : 1 Nov 2016 21:44
Operator : UM/SJ
Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

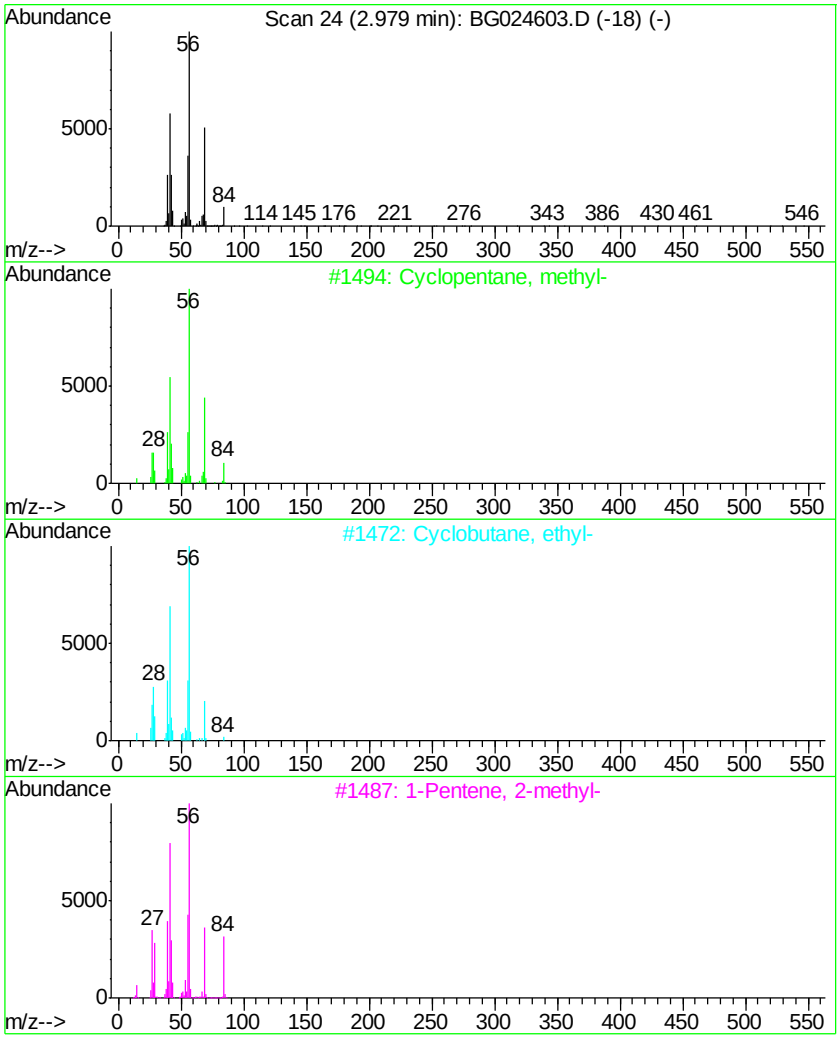
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

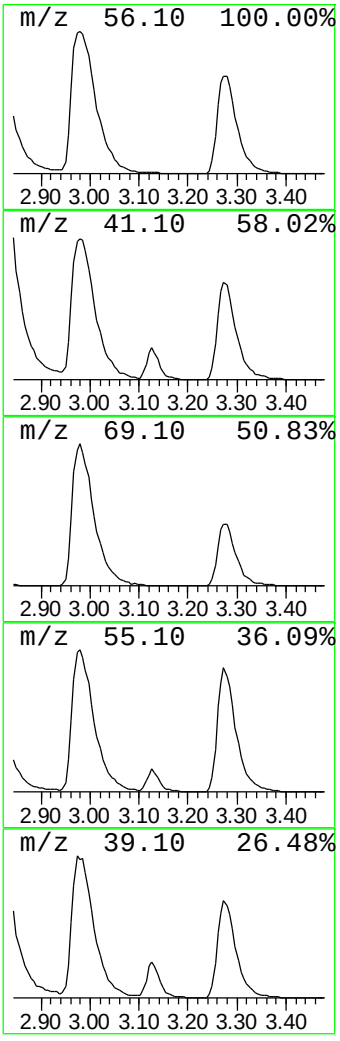
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	498.59 ng	20258900	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4	Cyclobutane	56	C4H8	000287-23-0	52
5	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	46





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024603.D
Acq On : 1 Nov 2016 21:44
Operator : UM/SJ
Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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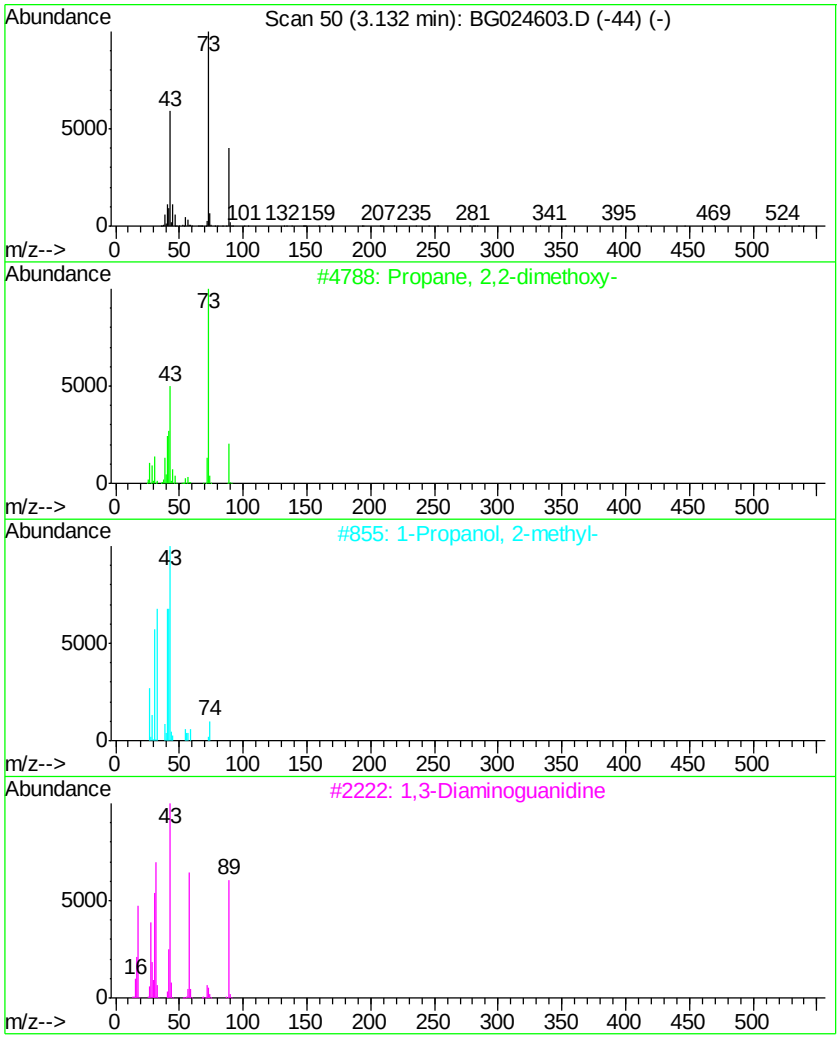
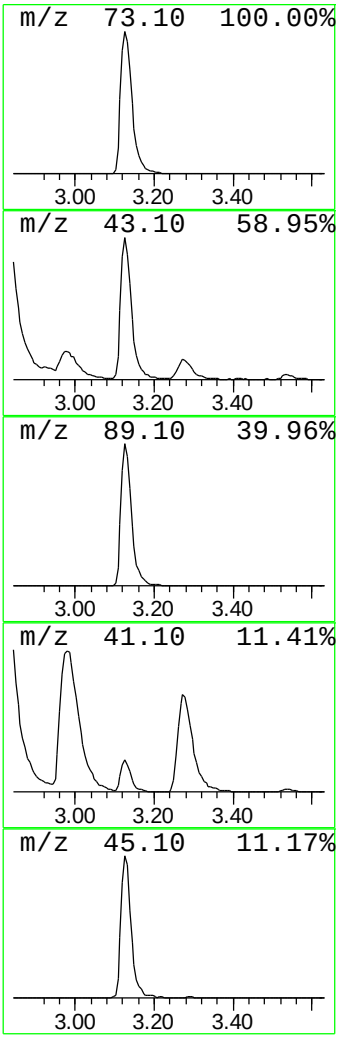
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	214.84 ng	8729660	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024603.D
Acq On : 1 Nov 2016 21:44
Operator : UM/SJ
Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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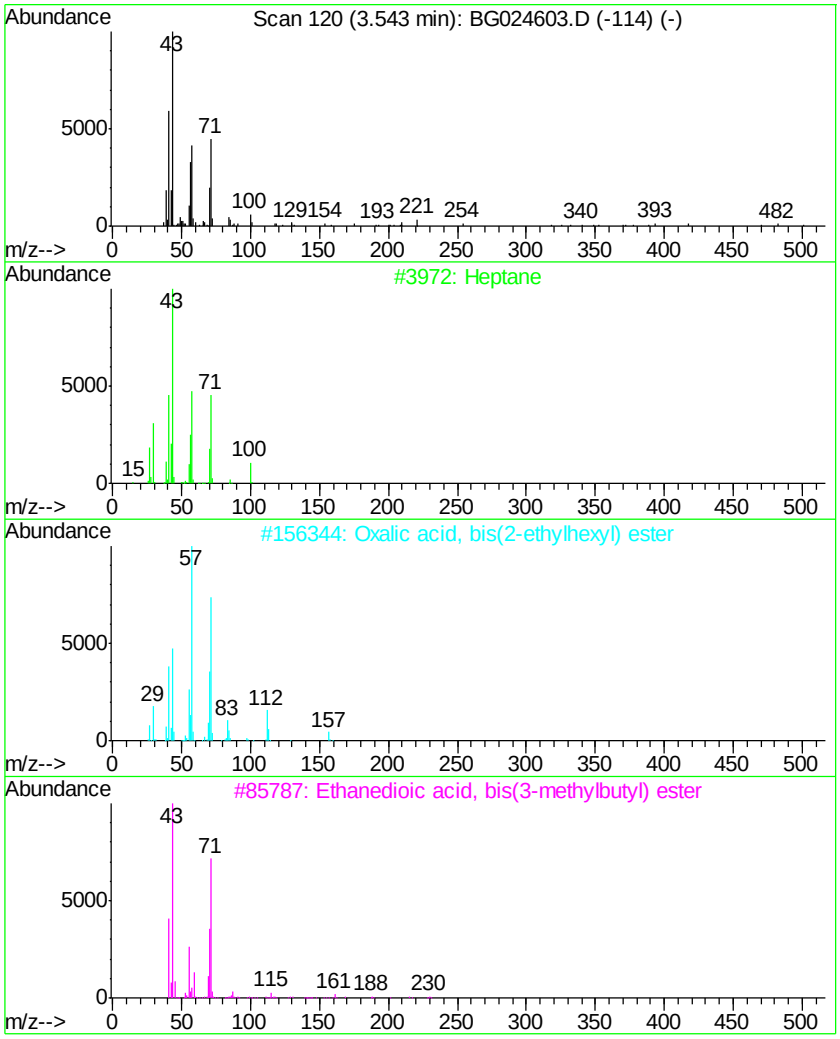
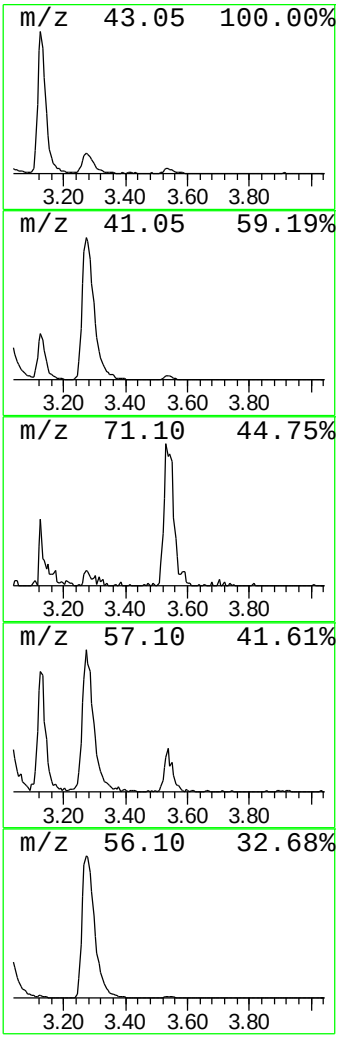
Peak Number 4 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	6.34 ng	257498	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	64
2	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	47
3	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	43
4	Decane, 2-methyl-	156	C11H24	006975-98-0	40
5	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	37





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Data File : BG024603.D
Acq On : 1 Nov 2016 21:44
Operator : UM/SJ
Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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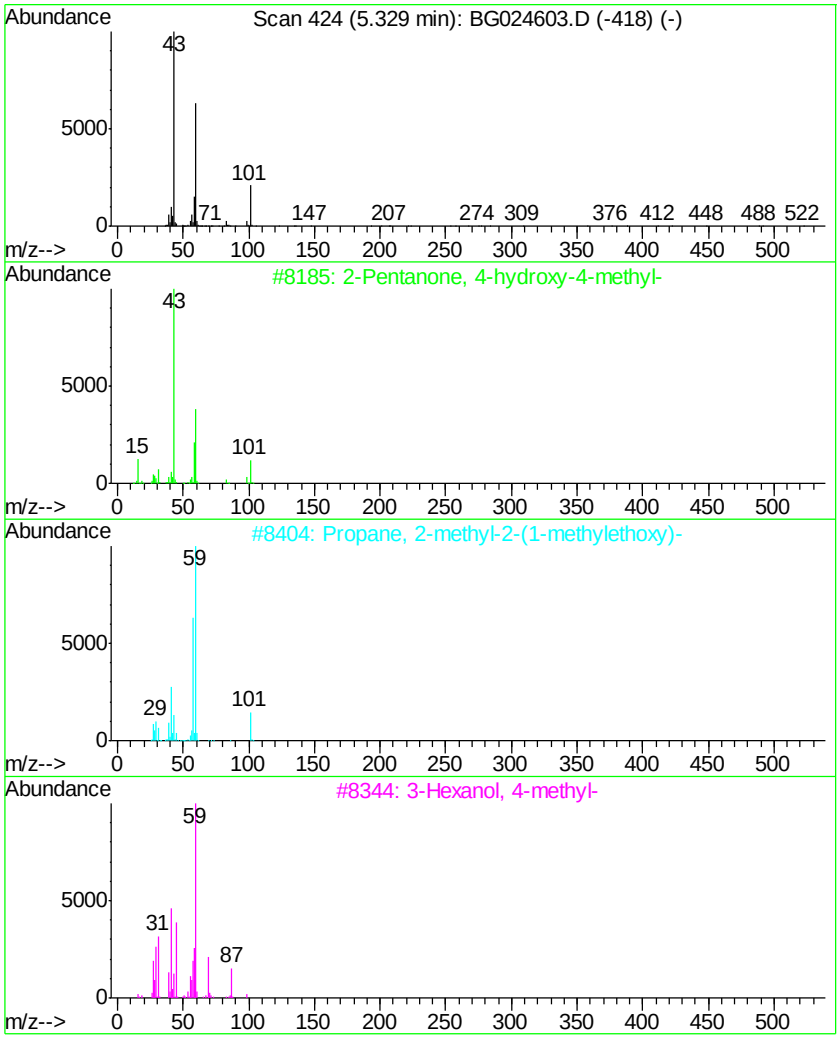
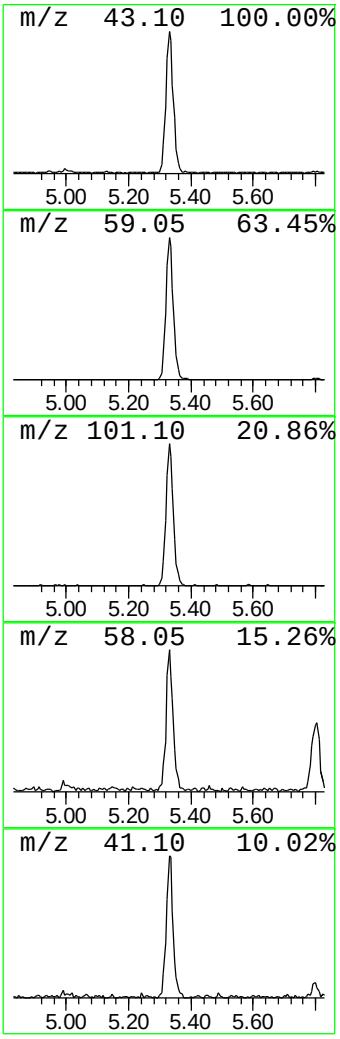
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	26.61 ng	1081080	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : H5489-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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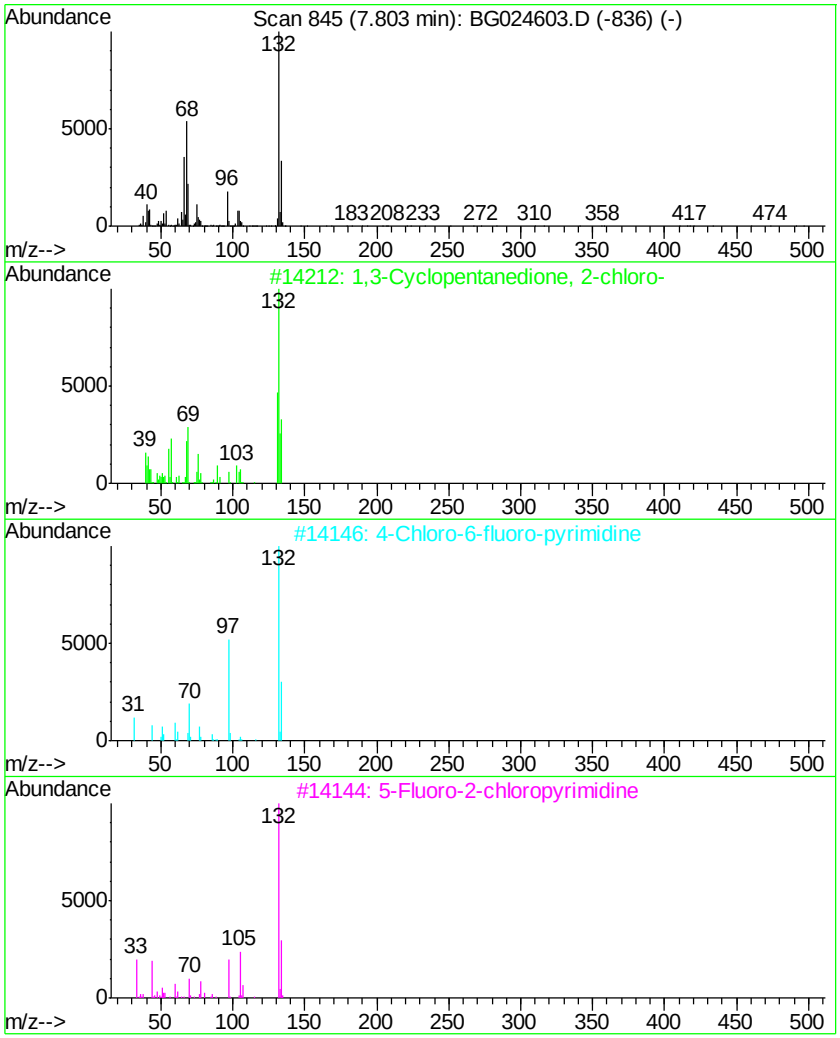
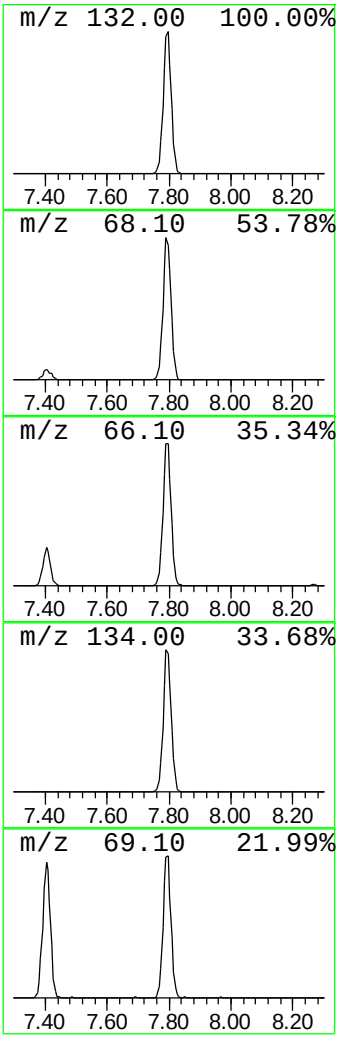
Peak Number 6 unknown7.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	125.69 ng	5107230	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	28
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16





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Instrument : BNA_G
ClientSampleId : SB-71-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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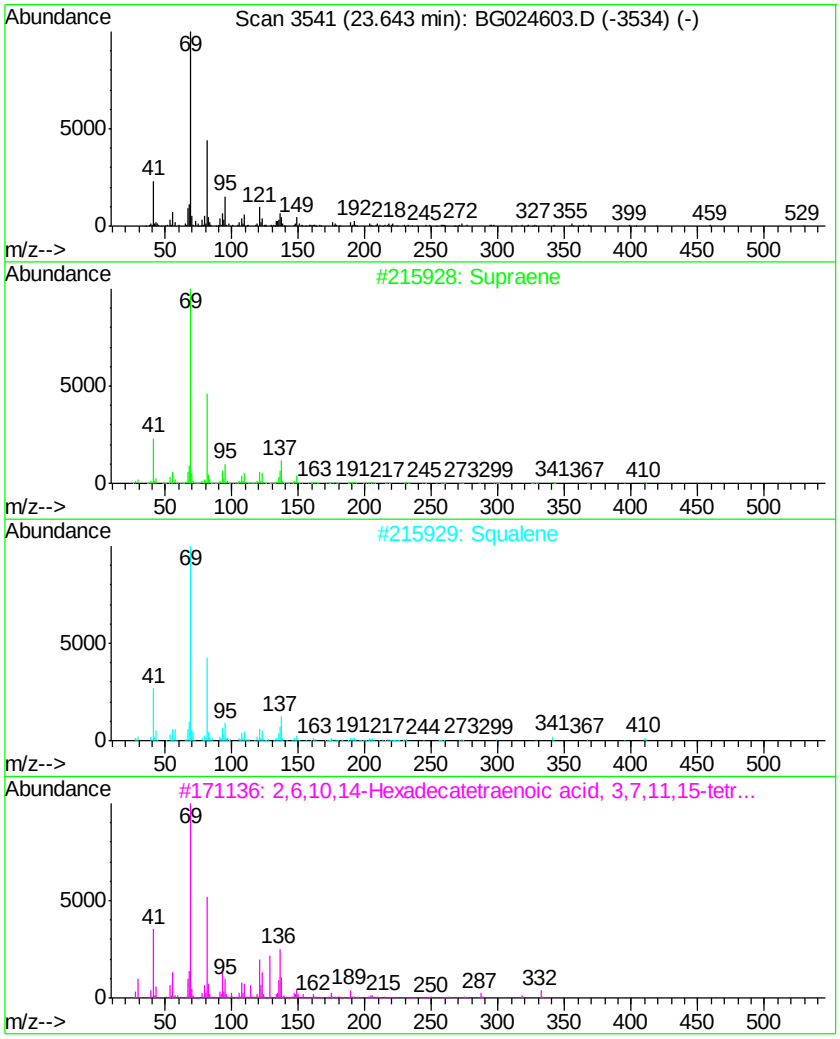
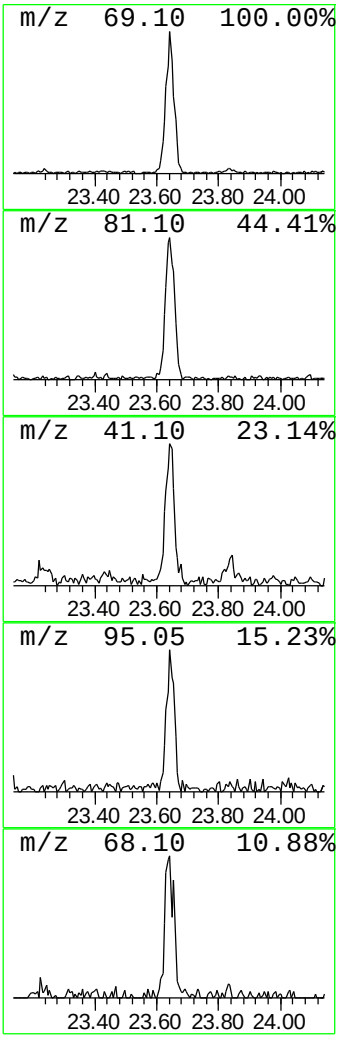
Peak Number 8 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	3.57 ng	505585	Perylene-d12	25.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	Squalene	410	C30H50	000111-02-4	72
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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
Cyclopentane, met...	2.98	498.6	ng	20258900	1	8.27	812655	20.0
Propane, 2,2-dime...	3.13	214.8	ng	8729660	1	8.27	812655	20.0
Heptane	3.54	6.3	ng	257498	1	8.27	812655	20.0
2-Pentanone, 4-hy...	5.33	26.6	ng	1081080	1	8.27	812655	20.0
unknown7.80	7.80	125.7	ng	5107230	1	8.27	812655	20.0
Supraene	23.64	3.6	ng	505585	6	25.35	2835520	20.0