LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG100317\
Data File : BG029014.D
Acq On : 3 Oct 2017 20:40
Operator : SJ/JU
Sample : PB102887BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

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-BG091217.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	4.140	88	94	103	rVB	98611	149210	3.92%	0.862%
2	4.739	190	196	204	rBV	135863	220499	5.79%	1.274%
3	4.845	209	214	226	rVB2	56161	94270	2.47%	0.544%
4	5.333	289	297	305	rBV	73502	118867	3.12%	0.687%
5	5.809	371	378	390	rBV	857866	1430482	37.54%	8.262%
6	7.325	629	636	642	rBV2	45826	69986	1.84%	0.404%
7	7.401	642	649	667	rVV2	717715	1330241	34.91%	7.683%
8	7.771	705	712	723	rBV	778943	1427195	37.45%	8.243%
9	8.241	785	792	803	rVB	164804	288831	7.58%	1.668%
10	8.564	840	847	855	rVB	603890	1061954	27.87%	6.134%
11	9.410	981	991	1003	rBV	479182	903623	23.71%	5.219%
12	11.061	1263	1272	1279	rBV	200774	389298	10.22%	2.248%
13	13.482	1677	1684	1694	rBV	1404548	2203464	57.82%	12.727%
14	14.863	1912	1919	1933	rVB2	241287	406168	10.66%	2.346%
15	16.355	2161	2173	2185	rBV	1193731	1955105	51.31%	11.292%
16	17.613	2379	2387	2395	rBV	497820	803228	21.08%	4.639%
17	20.204	2822	2828	2837	rBV	2989028	3810620	100.00%	22.009%
18	21.925	3114	3121	3130	rBV2	354568	650656	17.07%	3.758%

Sum of corrected areas: 17313697

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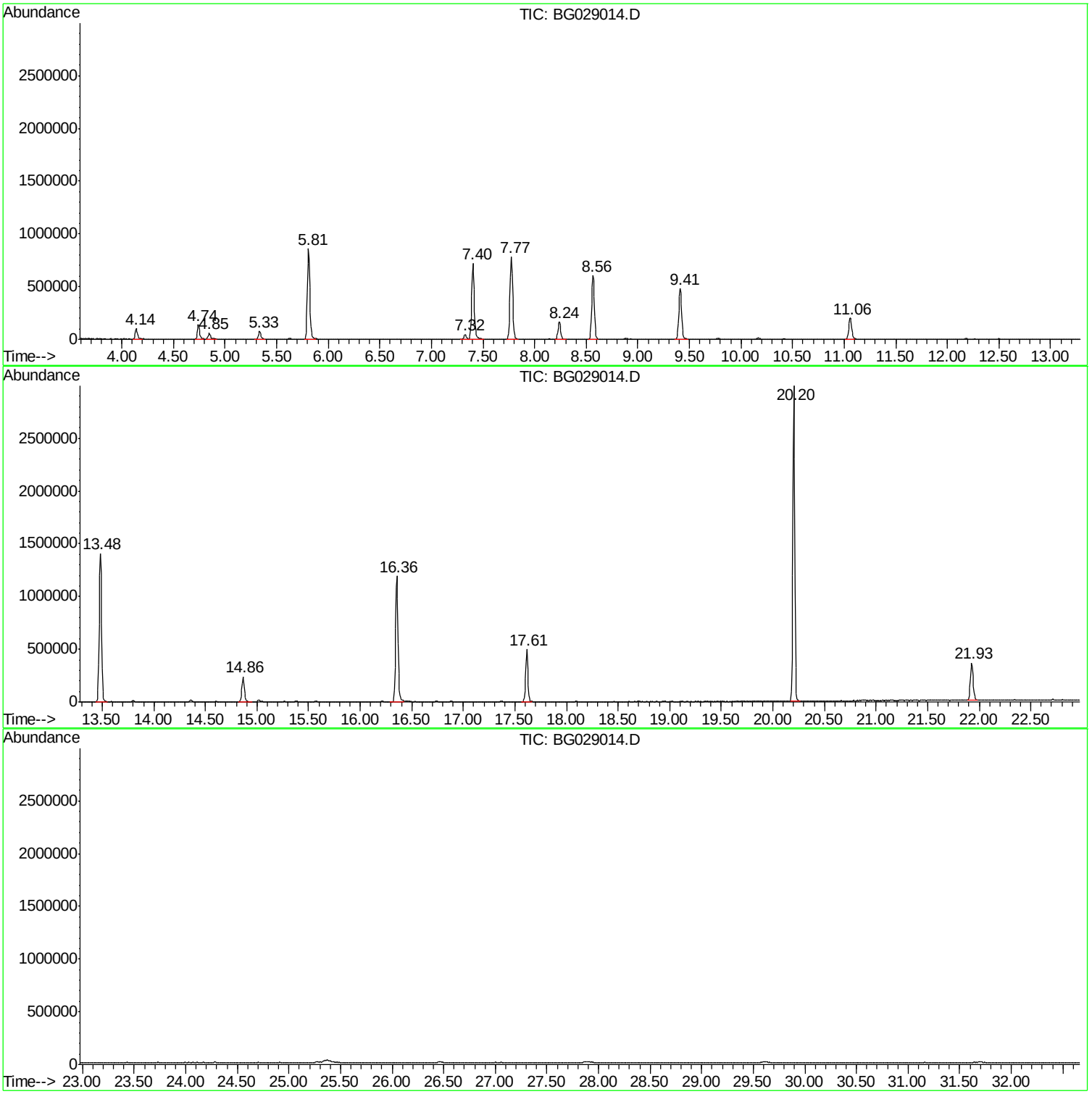
Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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Data File : BG029014.D
Acq On : 3 Oct 2017 20:40
Operator : SJ/JU
Sample : PB102887BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

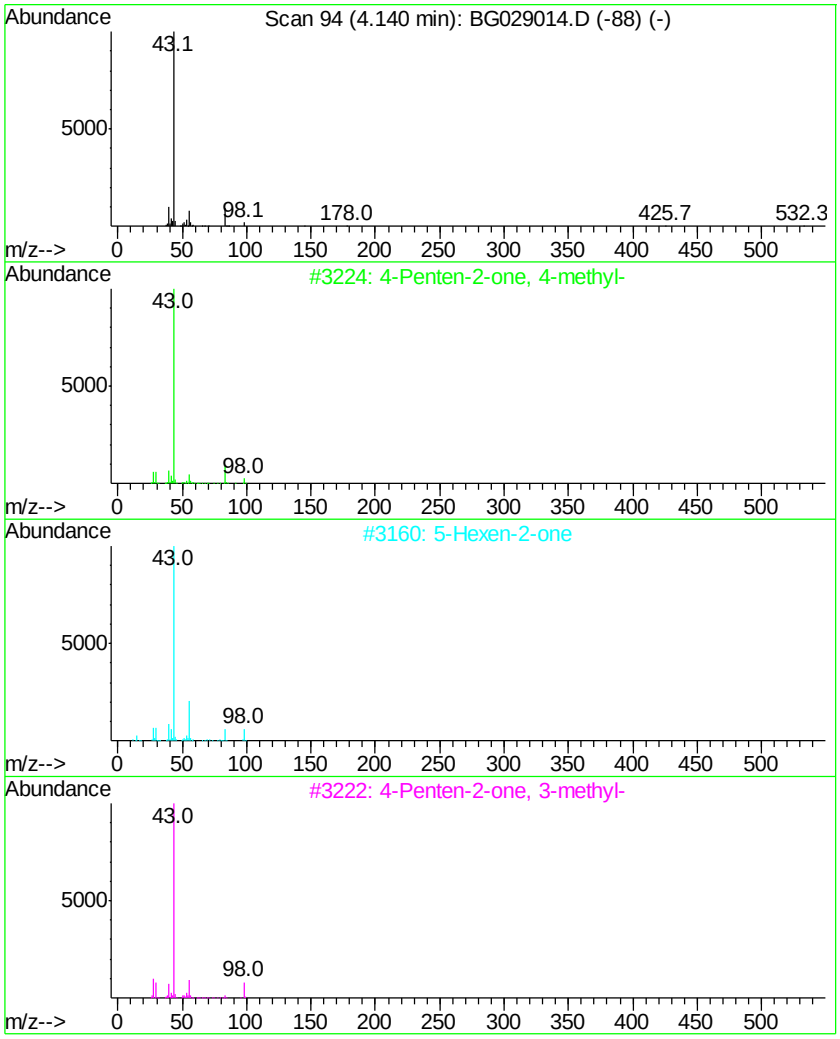
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

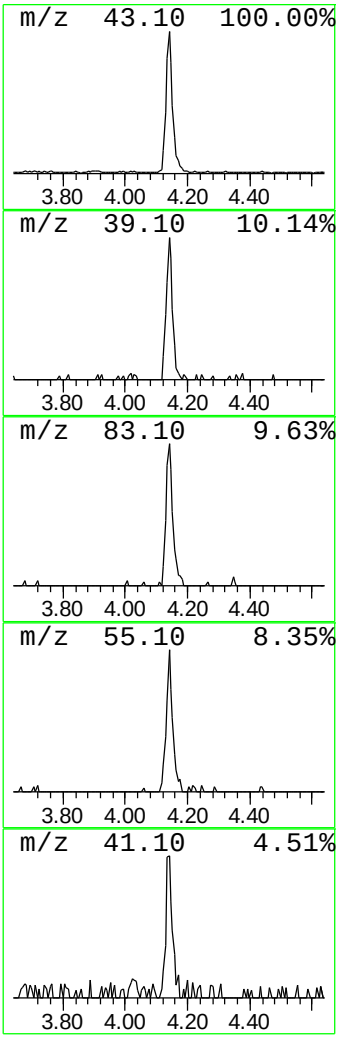
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	10.33 ng	149210	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	53
2	5-Hexen-2-one	98	C6H10O	000109-49-9	25
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
4	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	17
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10





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Data File : BG029014.D
Acq On : 3 Oct 2017 20:40
Operator : SJ/JU
Sample : PB102887BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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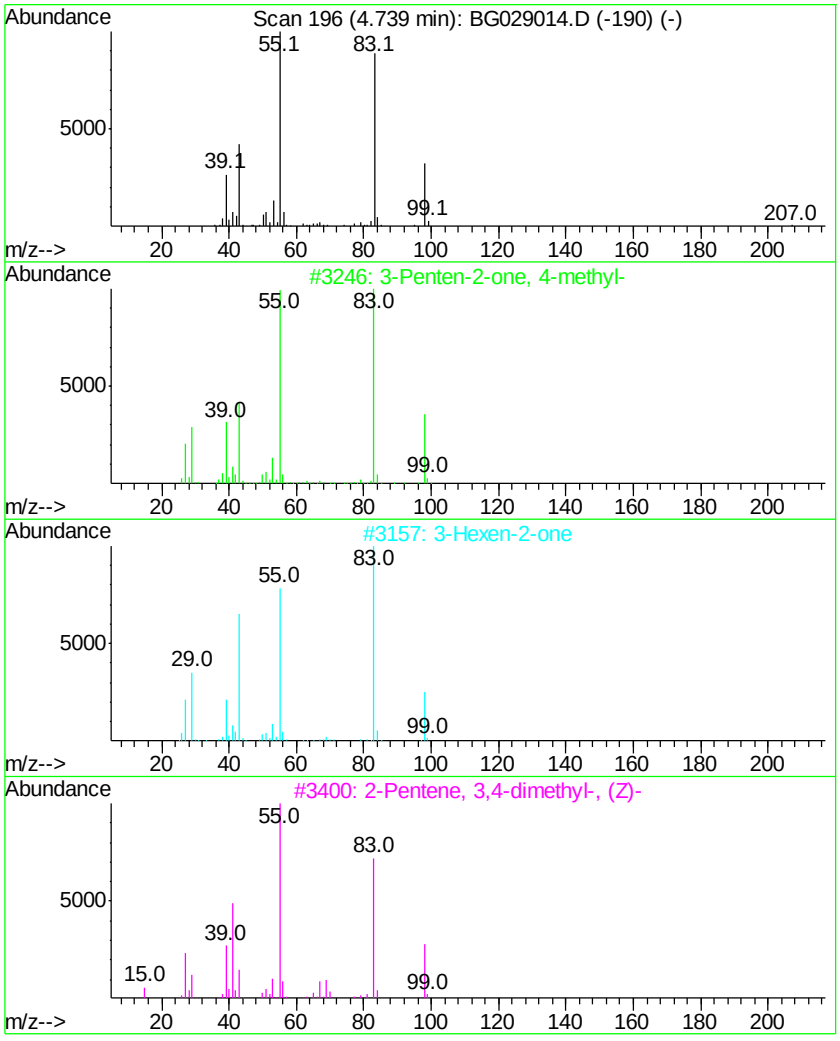
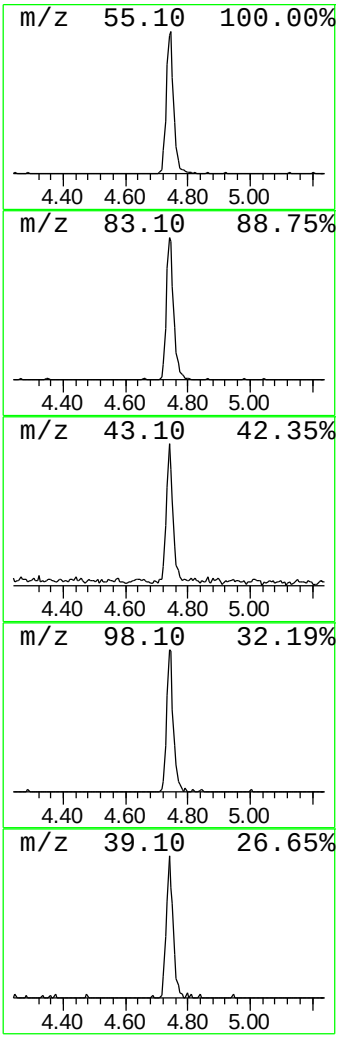
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	15.27 ng	220499	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	91
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	91
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG100317\
Data File : BG029014.D
Acq On : 3 Oct 2017 20:40
Operator : SJ/JU
Sample : PB102887BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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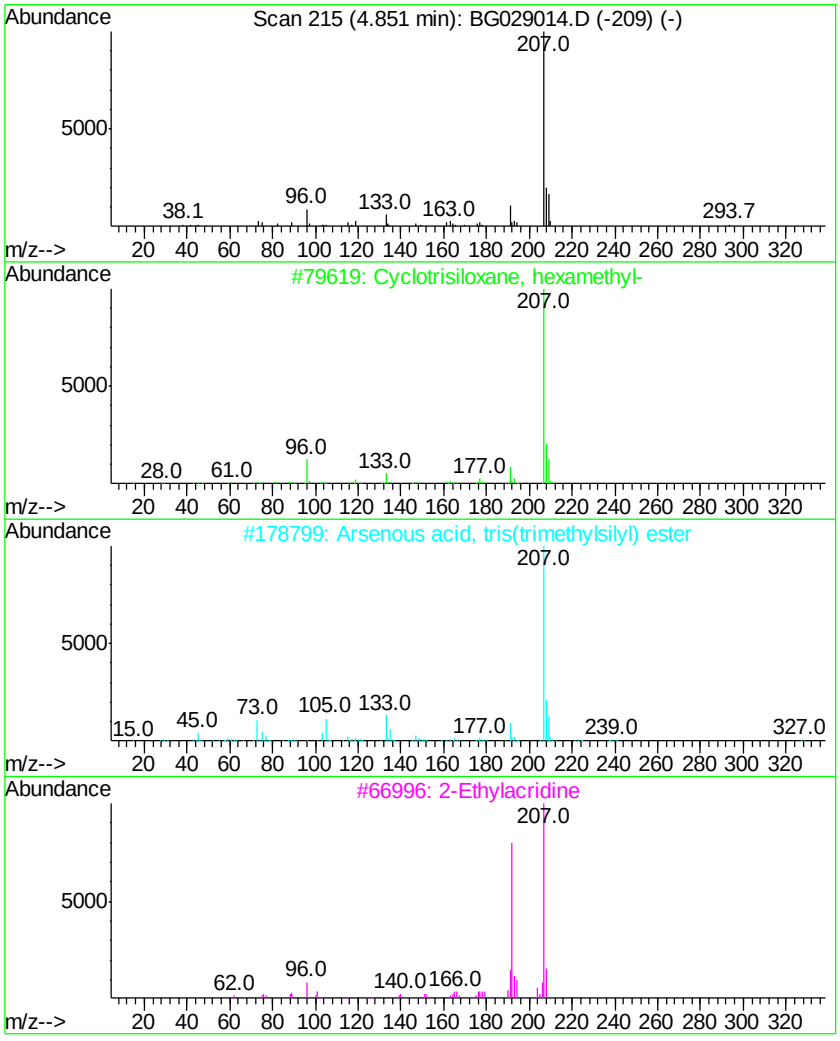
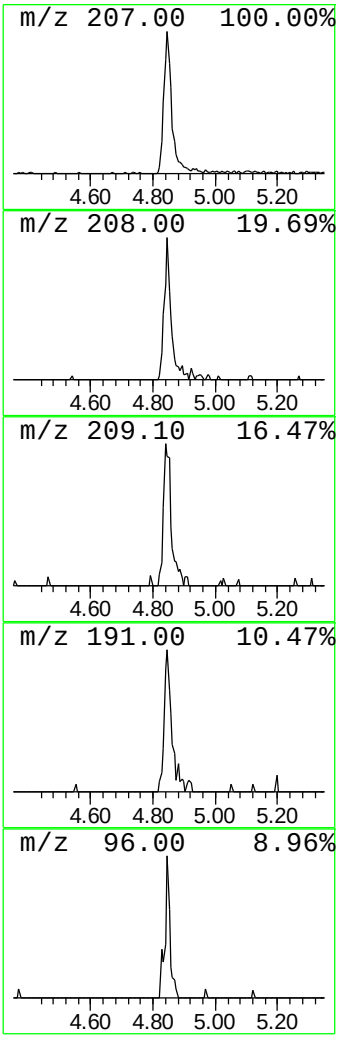
Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	6.53 ng	94270	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	90
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	56
3	2-Ethylacridine	207	C15H13N	055751-83-2	45
4	4-Cyclohexene-1,2-dicarboximide,...	207	C12H17NO2	028916-00-9	40
5	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	38





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Operator : SJ/JU
Sample : PB102887BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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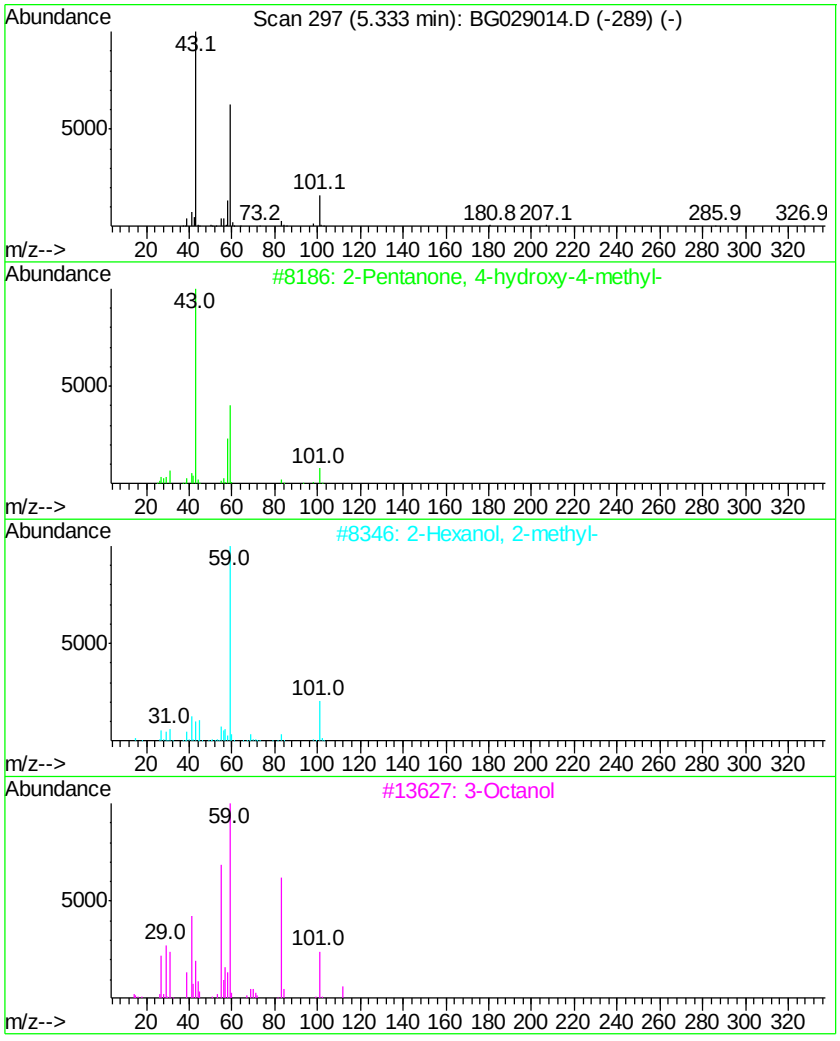
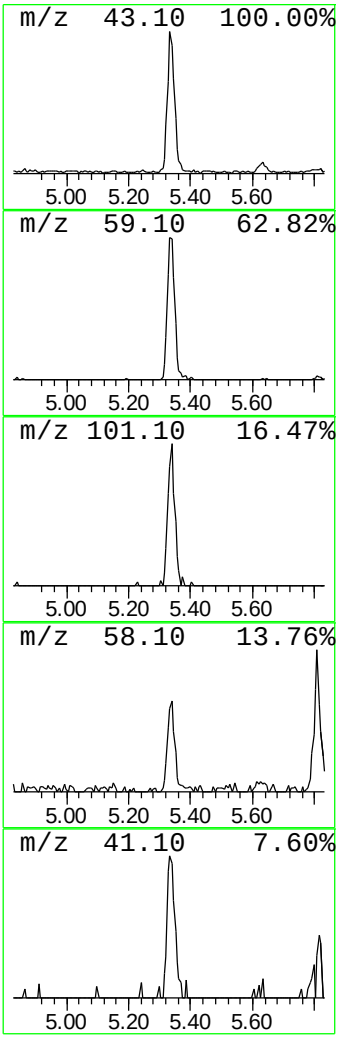
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	8.23 ng	118867	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50
3	3-Octanol	130	C8H18O	000589-98-0	36
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	33
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33





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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

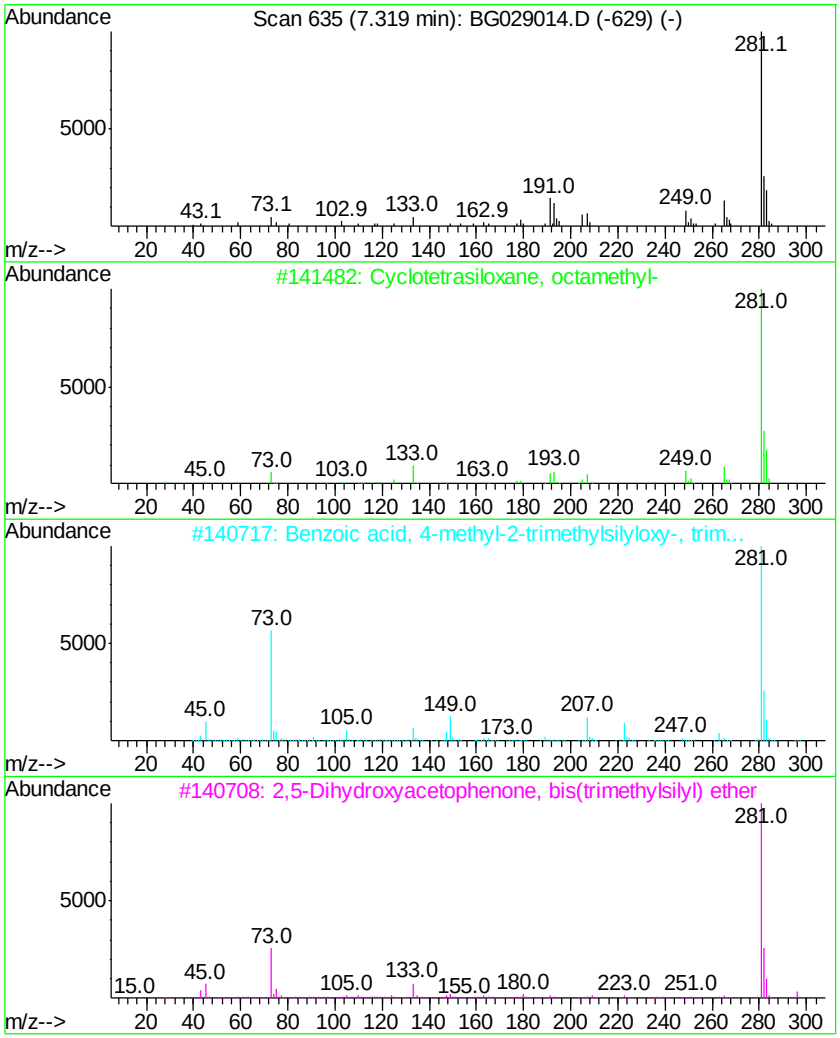
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

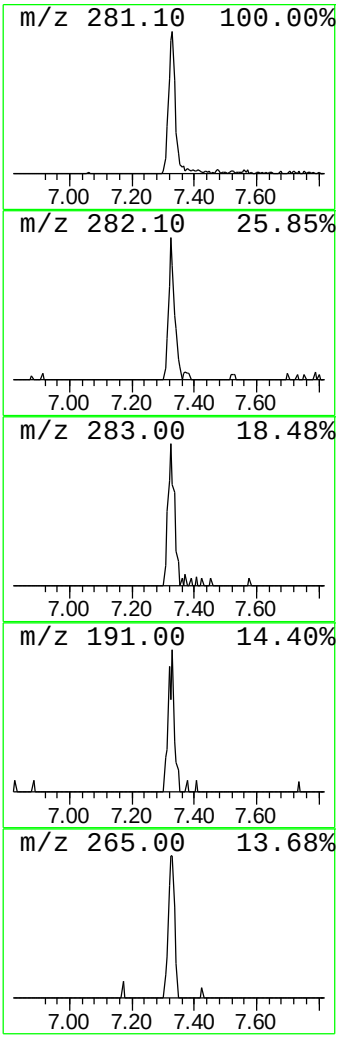
****

Peak Number 5 Cyclotetrasiloxane, octamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	4.85 ng	69986	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetrasiloxane, octamethyl-	296	C8H24O4Si4	000556-67-2	91
2	Benzoic acid, 4-methyl-2-trimeth...	296	C14H24O3Si2	1000153-59-3	59
3	2,5-Dihydroxyacetophenone, bis(t...	296	C14H24O3Si2	1000352-83-7	53
4	Benzene, 1-phenyl-4-(2-cyano-2-p...	281	C21H15N	027869-56-3	42
5	2',4'-Dihydroxyacetophenone, bis...	296	C14H24O3Si2	1000352-82-1	40





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB102887BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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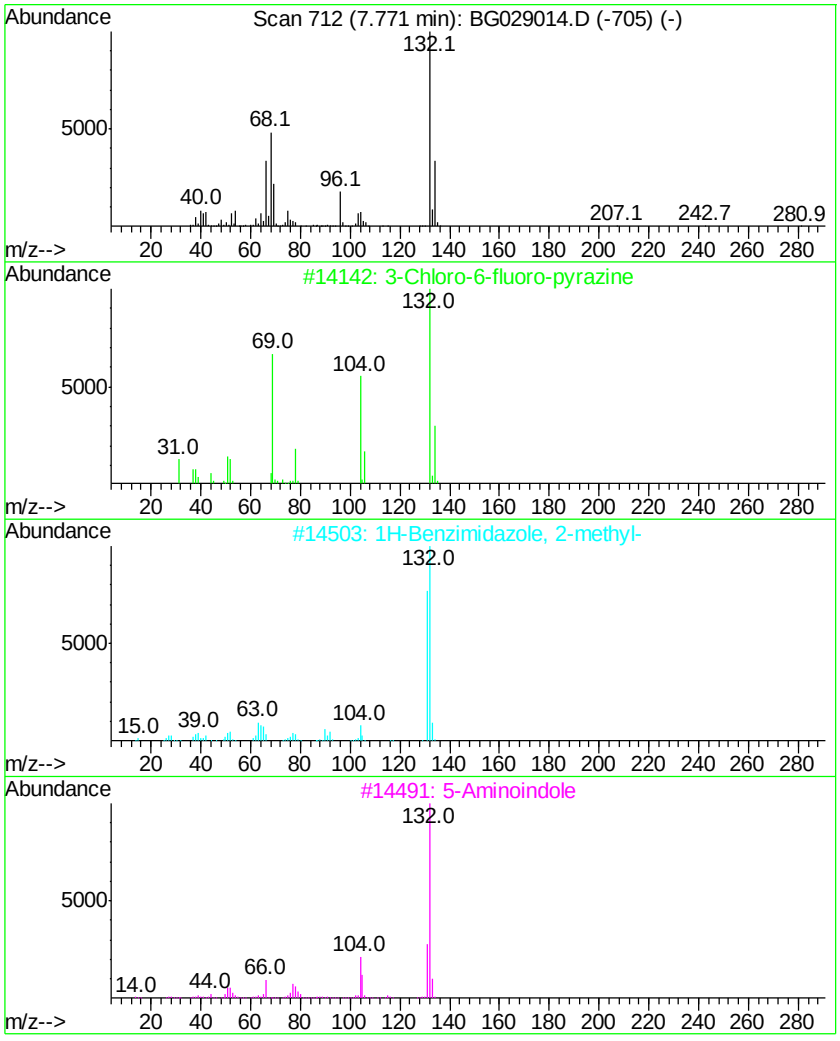
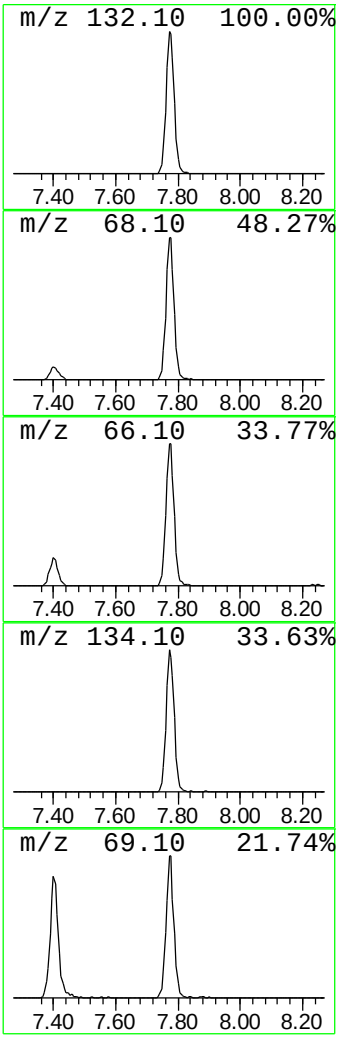
Peak Number 6 unknown7.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.77	98.83 ng	1427200	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Tentatively Identified Compound (LSC) summary

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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...	4.14	10.3	ng	149210	1	8.24	288831	20.0
3-Penten-2-one, 4...	4.74	15.3	ng	220499	1	8.24	288831	20.0
Cyclotrisiloxane,...	4.85	6.5	ng	94270	1	8.24	288831	20.0
2-Pentanone, 4-hy...	5.33	8.2	ng	118867	1	8.24	288831	20.0
Cyclotetrasiloxan...	7.32	4.8	ng	69986	1	8.24	288831	20.0
unknown7.77	7.77	98.8	ng	1427200	1	8.24	288831	20.0