LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060917\
Data File : BG027366.D
Acq On : 10 Jun 2017 3:20
Operator : SJ/MA
Sample : I3566-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-01-COMP(0-10)

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-BG060517.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	4.551	142	147	156	rBV	37379	66018	2.12%	0.361%
2	5.127	239	245	255	rVB	27256	49027	1.57%	0.268%
3	5.697	336	342	354	rBV	246123	423256	13.59%	2.312%
4	6.143	410	418	434	rVB	764706	1369291	43.96%	7.480%
5	7.688	673	681	693	rVB	853929	1614256	51.83%	8.818%
6	8.088	741	749	760	rBV	792972	1446384	46.44%	7.901%
7	8.552	821	828	838	rBV	158756	292971	9.41%	1.600%
8	8.881	876	884	895	rVB	511947	961843	30.88%	5.254%
9	9.715	1016	1026	1040	rBV	471166	909880	29.21%	4.971%
10	11.372	1300	1308	1320	rVB	257144	491937	15.79%	2.687%
11	13.758	1707	1714	1724	rBV	1405139	2246727	72.13%	12.273%
12	14.563	1845	1851	1858	rBV	162645	249346	8.01%	1.362%
13	15.133	1941	1948	1956	rVB2	433974	740684	23.78%	4.046%
14	15.932	2073	2084	2090	rBV	26407	38585	1.24%	0.211%
15	16.613	2194	2200	2210	rBV	986583	1578986	50.69%	8.626%
16	16.795	2226	2231	2240	rBV	28837	45658	1.47%	0.249%
17	17.882	2409	2416	2424	rBV2	581805	926236	29.74%	5.060%
18	20.462	2848	2855	2865	rBV	2218641	3114793	100.00%	17.016%
19	22.265	3154	3162	3172	rBV	480532	968277	31.09%	5.290%
20	25.955	3778	3790	3804	rBV3	205919	771408	24.77%	4.214%

Sum of corrected areas: 18305563

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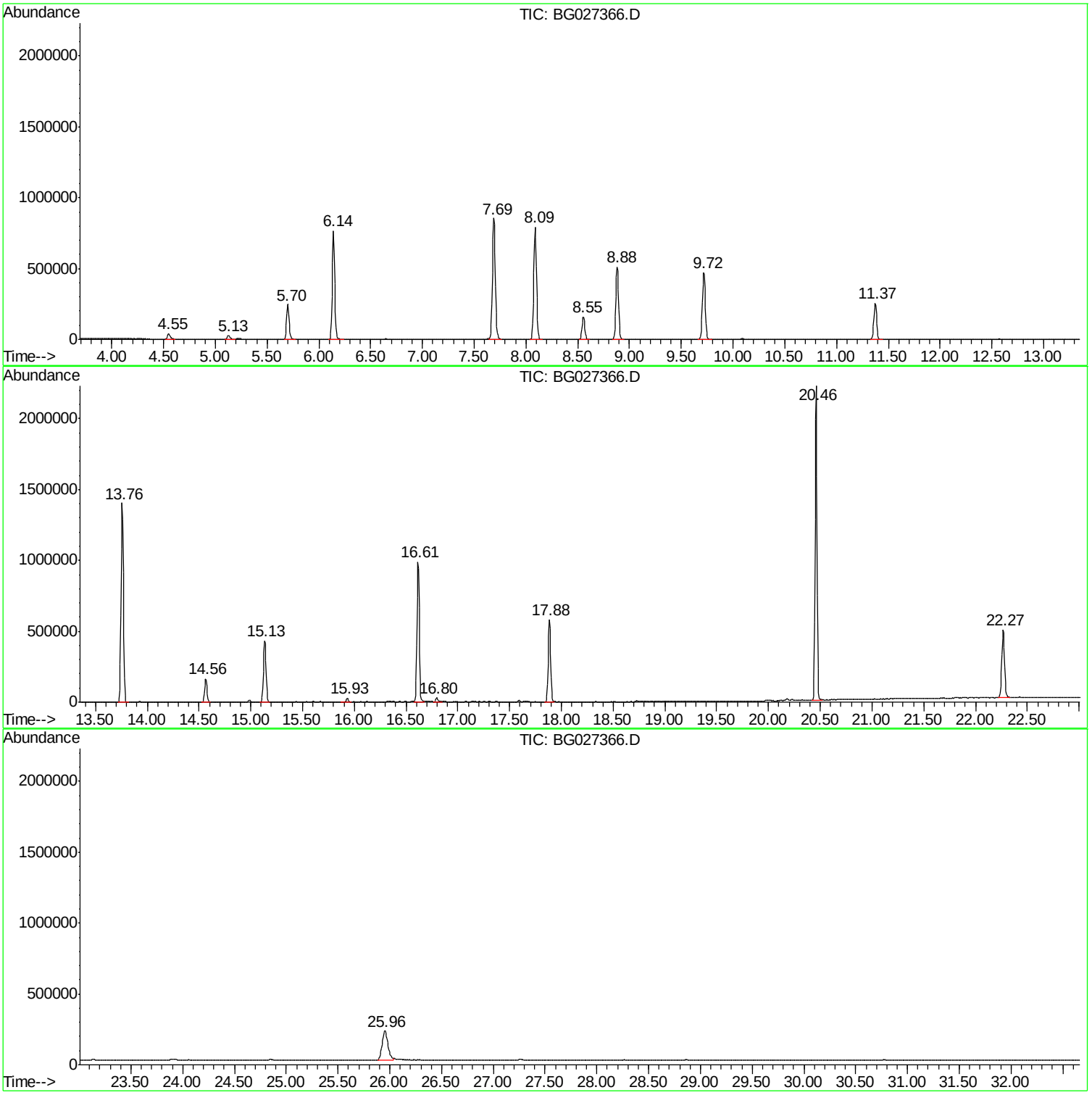
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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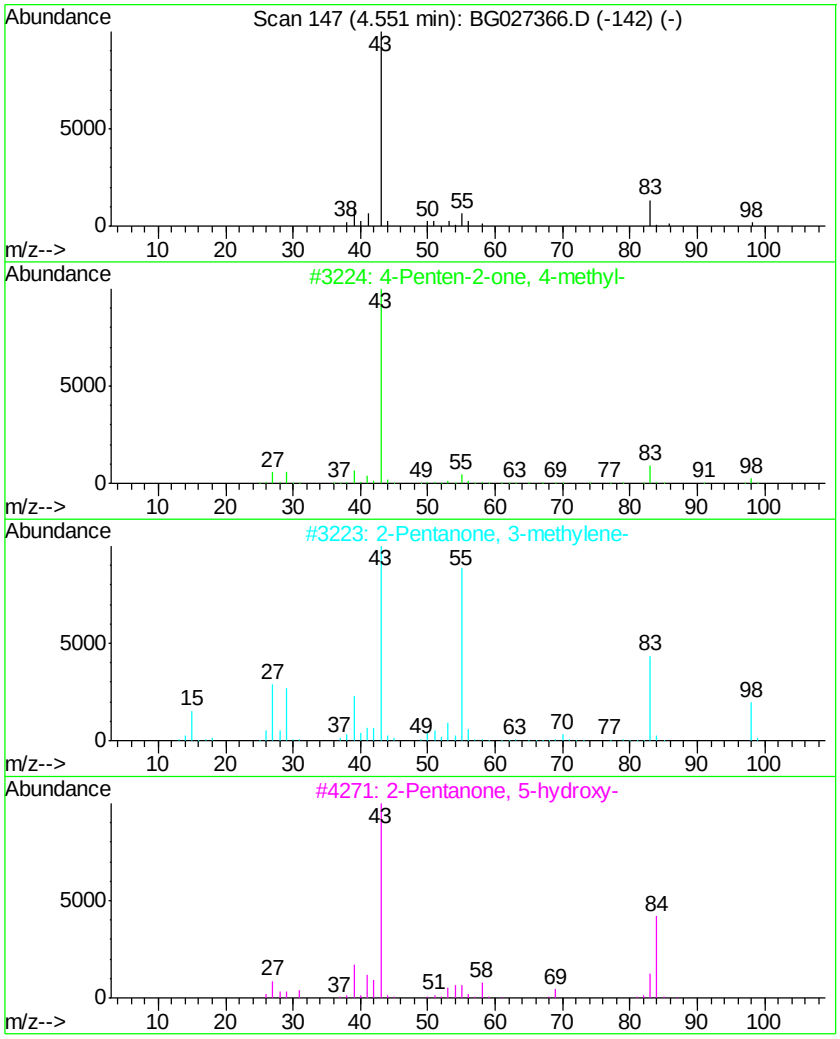
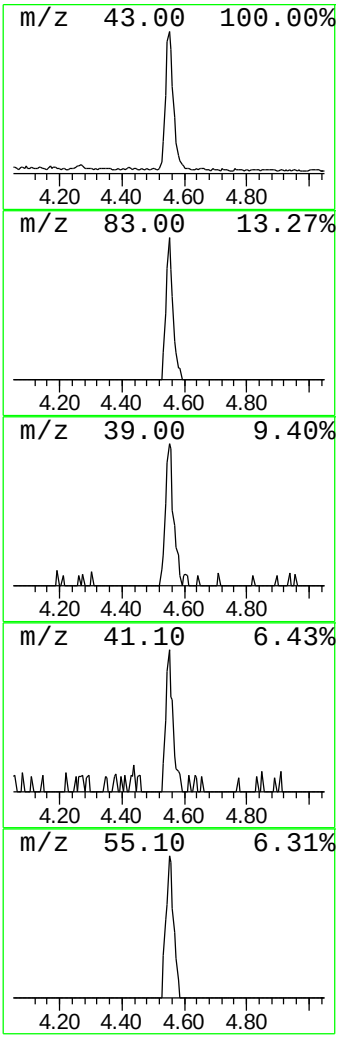
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	4.51 ng	66018	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9
3	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-01-COMP(0-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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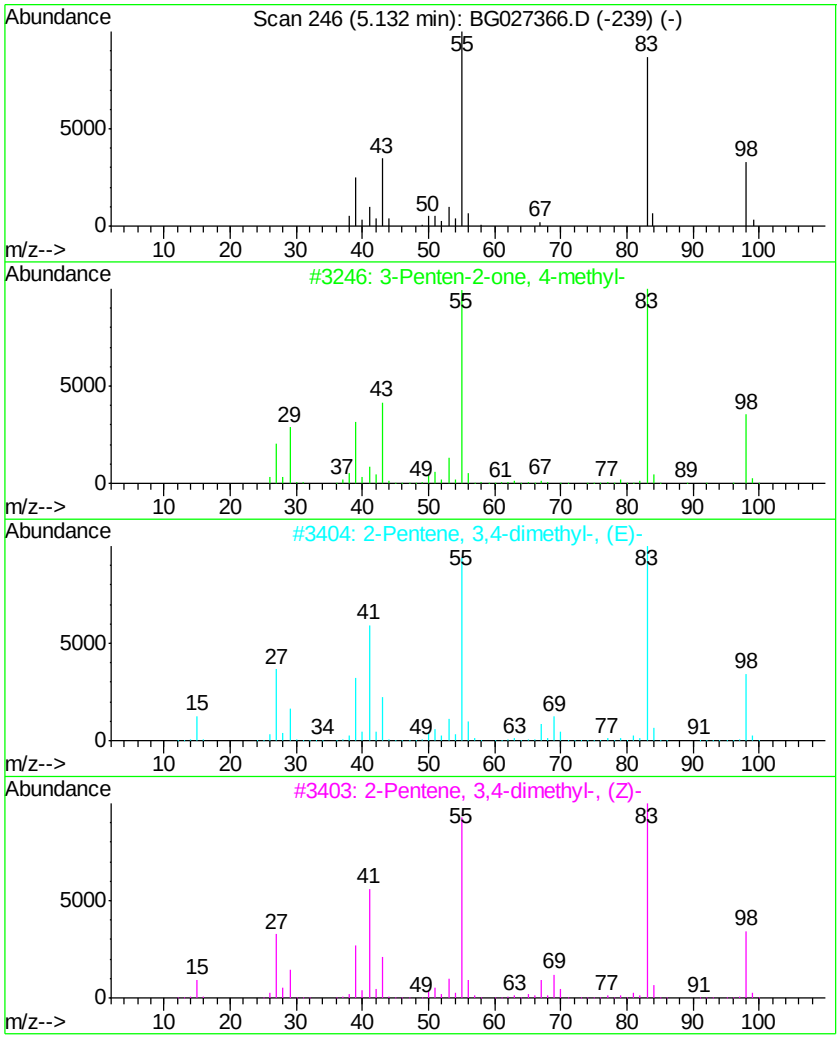
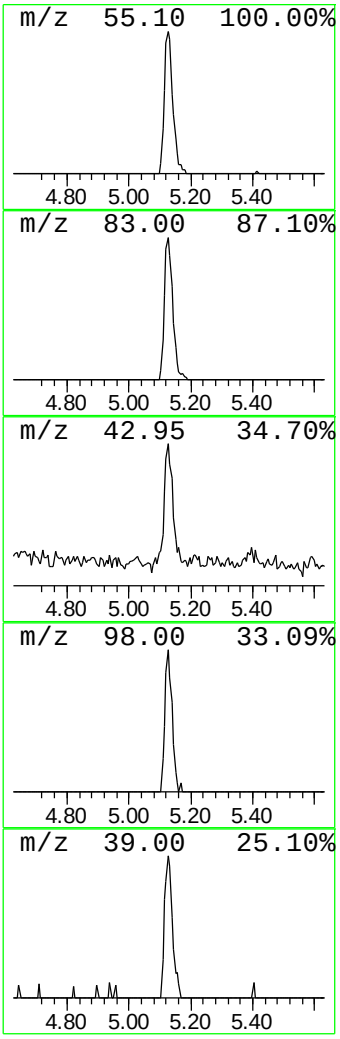
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.35 ng	49027	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	3-Hexen-2-one	98	C6H10O	000763-93-9	80
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	78





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-01-COMP(0-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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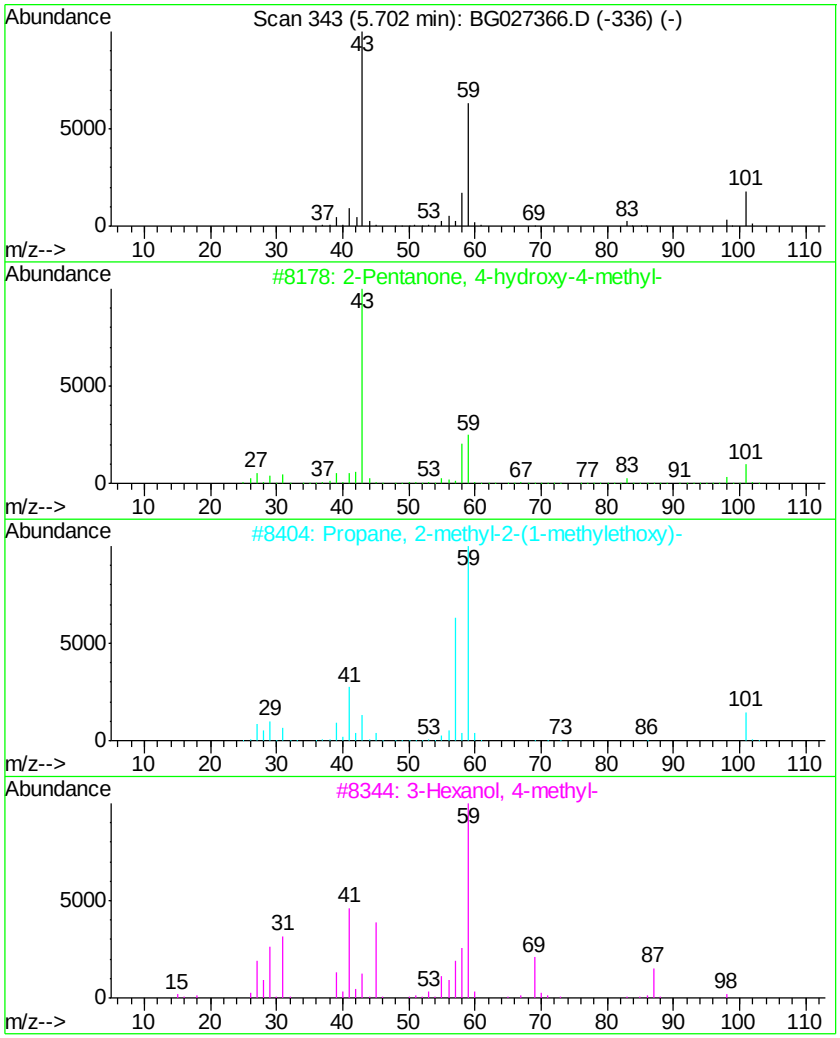
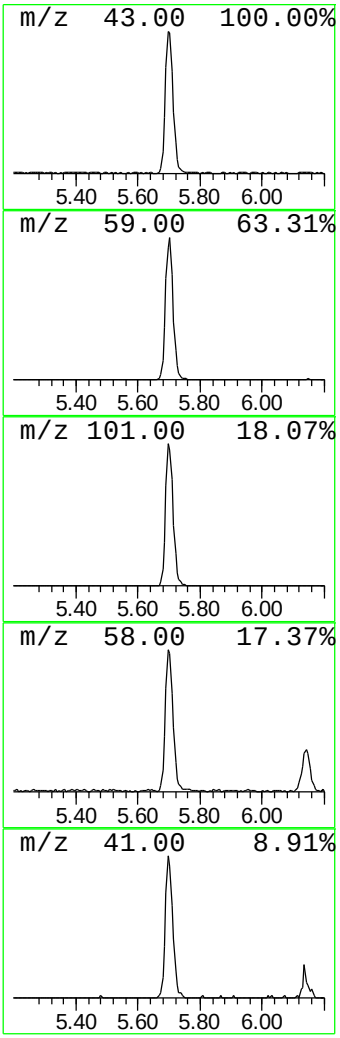
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	28.89 ng	423256	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	1,2-Butanediol	90	C4H10O2	000584-03-2	28





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-01-COMP(0-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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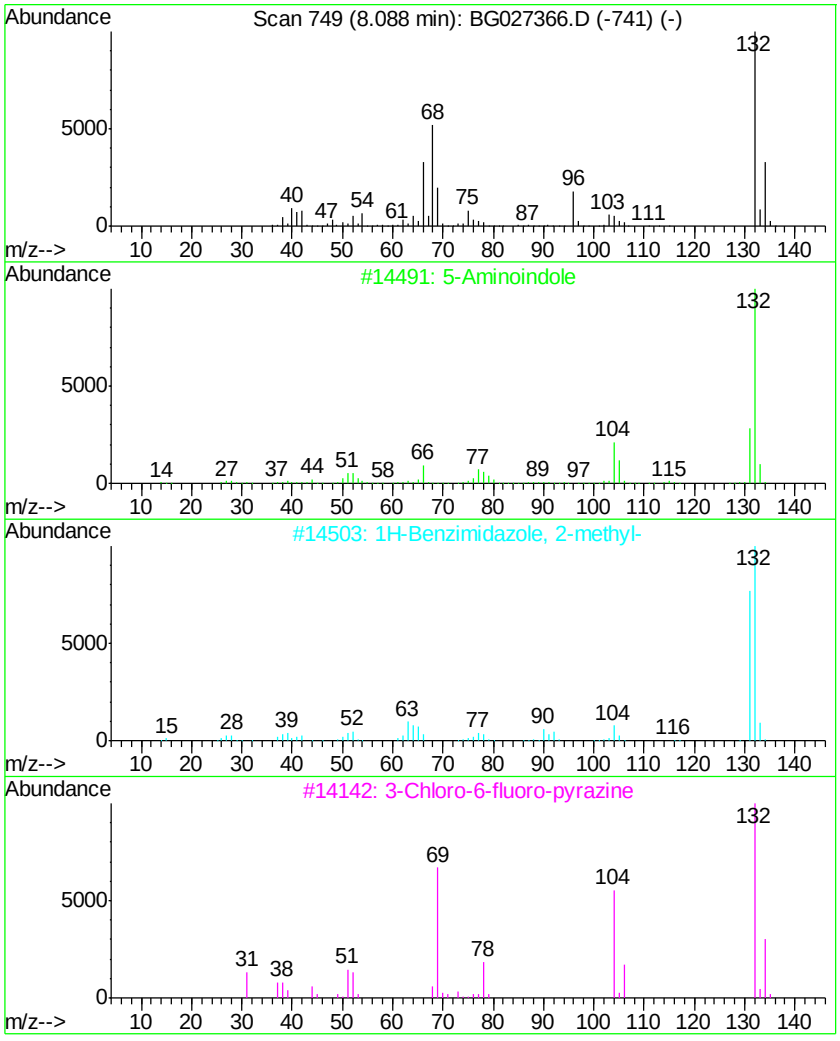
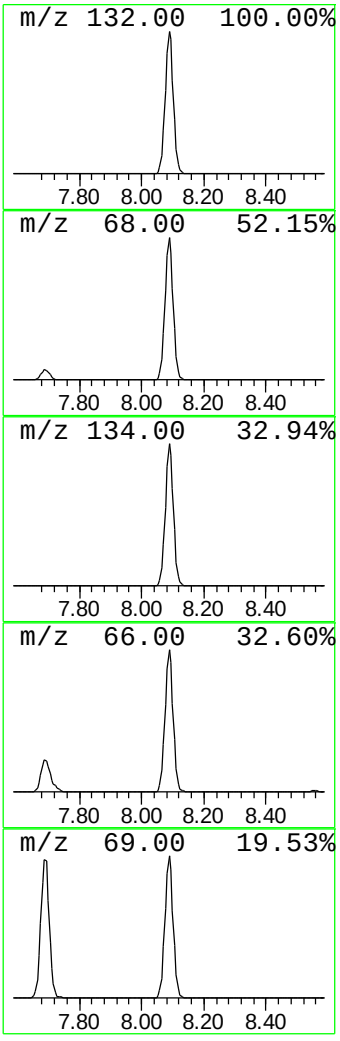
Peak Number 4 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	98.74 ng	1446380	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	16
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Penten-2-one, 4...	4.55	4.5	ng	66018	1	8.56	292971	20.0
3-Penten-2-one, 4...	5.13	3.4	ng	49027	1	8.56	292971	20.0
2-Pentanone, 4-hy...	5.70	28.9	ng	423256	1	8.56	292971	20.0
unknown8.09	8.09	98.7	ng	1446380	1	8.56	292971	20.0