LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023416.D
Acq On : 3 Aug 2016 4:22
Operator : UM/SJ
Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

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-BG080116.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	2.992	21	26	48	rVB	4844938	8486781	94.34%	13.779%
2	5.183	393	399	408	rBV	625685	982136	10.92%	1.595%
3	5.665	473	481	492	rBV	2246768	3703913	41.17%	6.014%
4	7.274	748	755	771	rBV	2399501	4377271	48.66%	7.107%
5	7.650	811	819	828	rBV	2277764	4020506	44.69%	6.528%
6	8.120	892	899	907	rBV	370244	668137	7.43%	1.085%
7	8.443	947	954	964	rBV	1478873	2684765	29.85%	4.359%
8	9.295	1092	1099	1110	rBV	1482005	2630074	29.24%	4.270%
9	10.951	1373	1381	1389	rBV	599461	1083405	12.04%	1.759%
10	13.395	1789	1797	1805	rBV	3854855	6314678	70.20%	10.253%
11	14.224	1932	1938	1944	rBV	615960	906491	10.08%	1.472%
12	14.782	2026	2033	2042	rBV2	1140672	1834196	20.39%	2.978%
13	15.604	2168	2173	2178	rVB	83682	109506	1.22%	0.178%
14	16.280	2281	2288	2297	rBV	4539708	6865104	76.32%	11.146%
15	16.468	2315	2320	2330	rVB	92763	161430	1.79%	0.262%
16	17.543	2496	2503	2511	rBV2	1655466	2537170	28.20%	4.119%
17	18.412	2645	2651	2660	rBV	171960	277352	3.08%	0.450%
18	20.151	2941	2947	2953	rBV	6683066	8995586	100.00%	14.606%
19	20.926	3075	3079	3085	rBV	188022	242974	2.70%	0.395%
20	21.854	3231	3237	3248	rVB2	1426559	2403813	26.72%	3.903%
21	25.238	3802	3813	3826	rVB2	774371	2305008	25.62%	3.742%

Sum of corrected areas: 61590296

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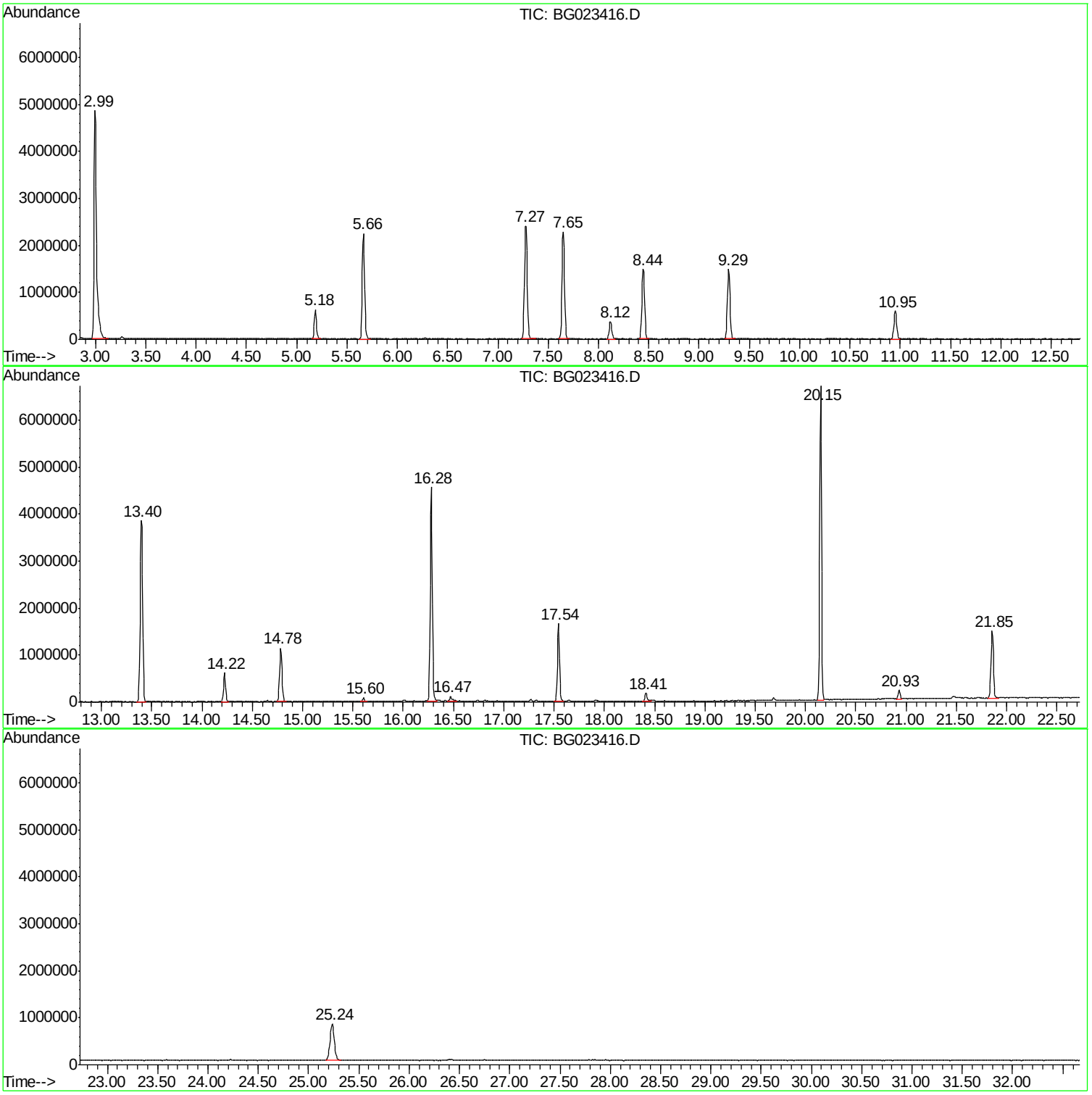
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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\BG080216\
Data File : BG023416.D
Acq On : 3 Aug 2016 4:22
Operator : UM/SJ
Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

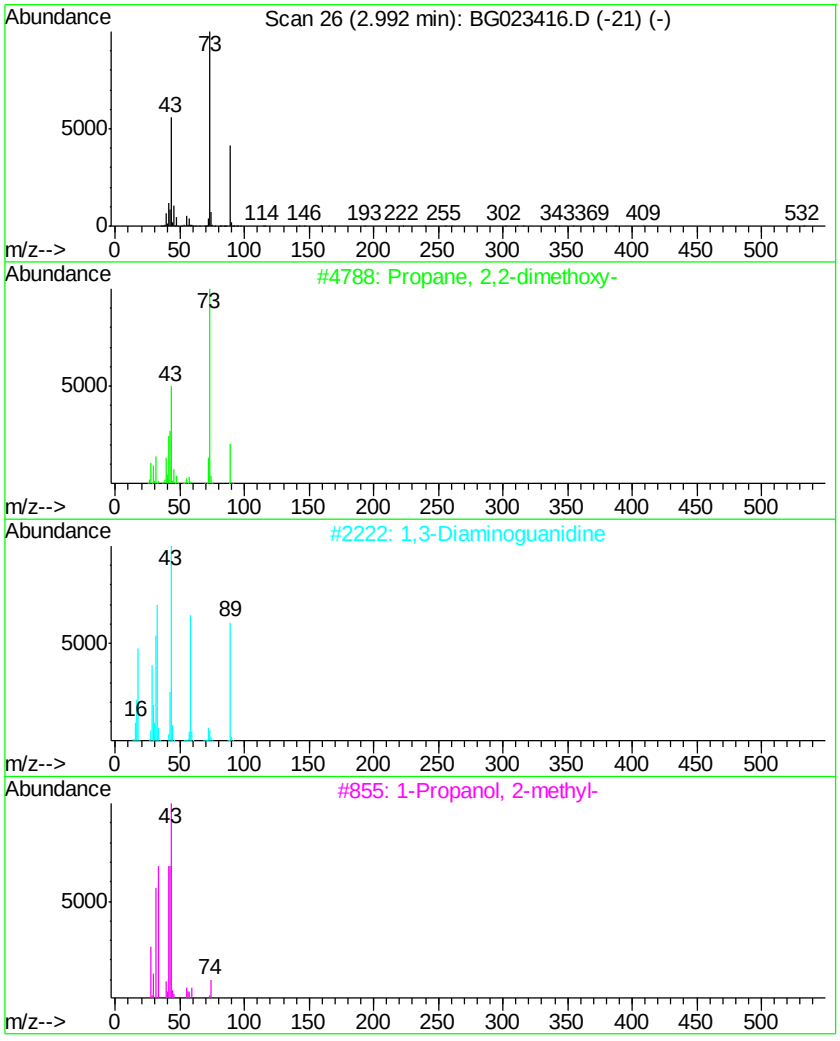
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

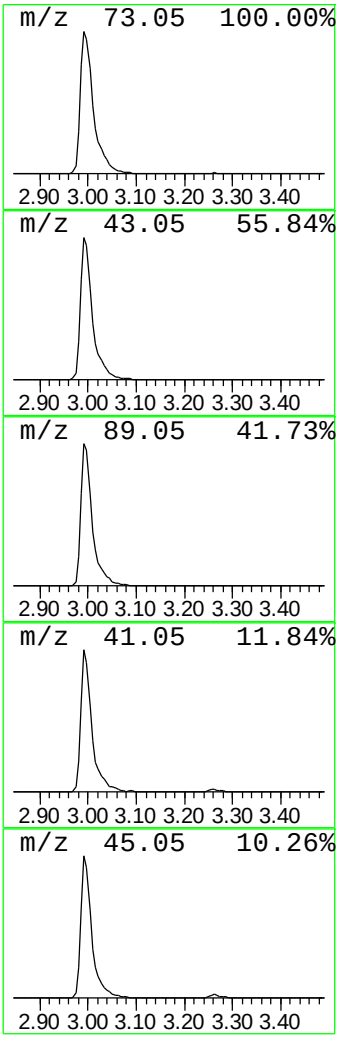
****

Peak Number 1 unknown2.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	254.04 ng	8486780	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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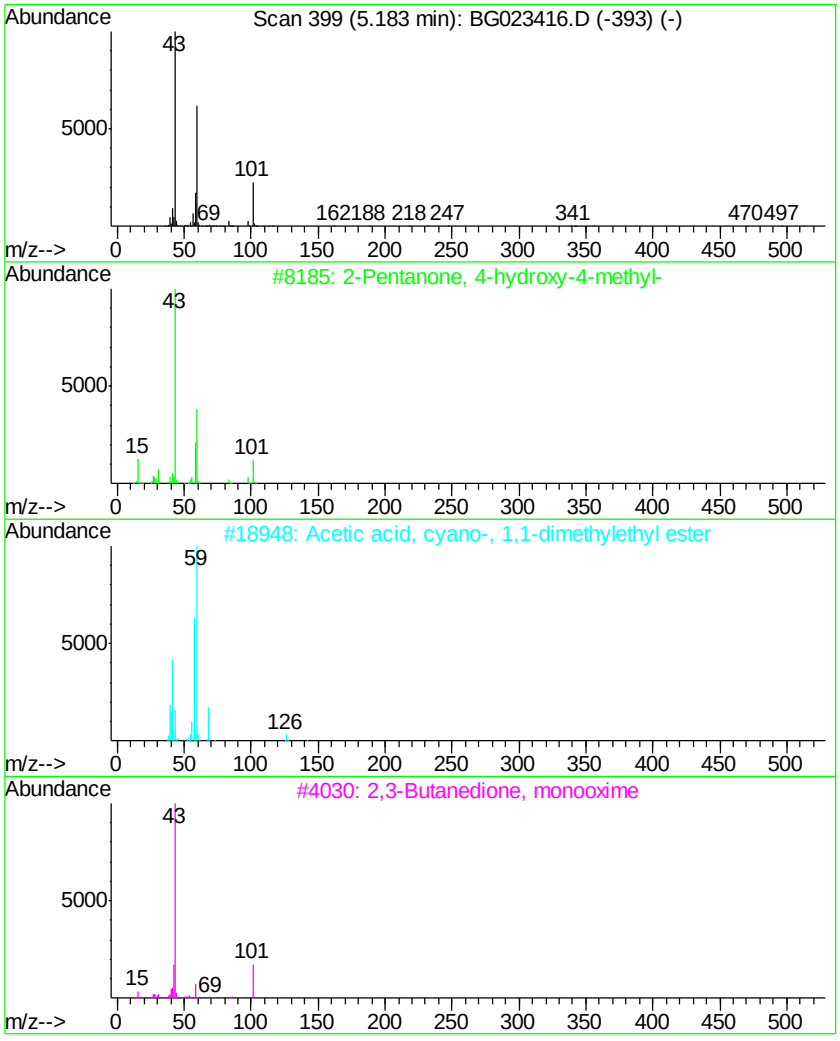
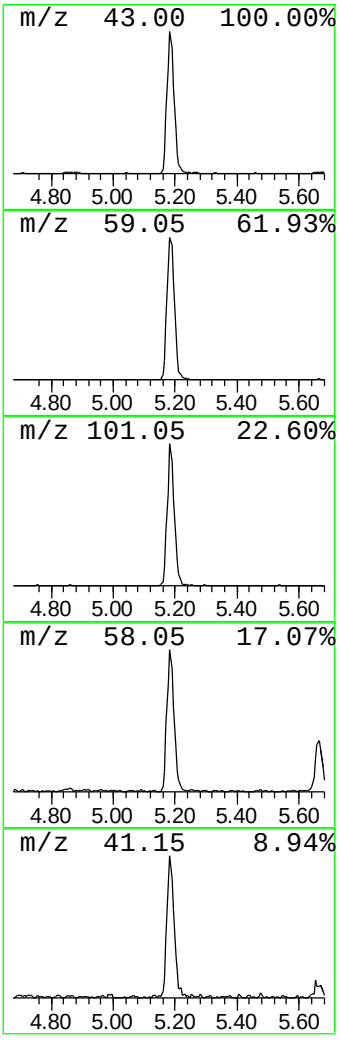
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	29.40 ng	982136	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 3 Aug 2016 4:22
Operator : UM/SJ
Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
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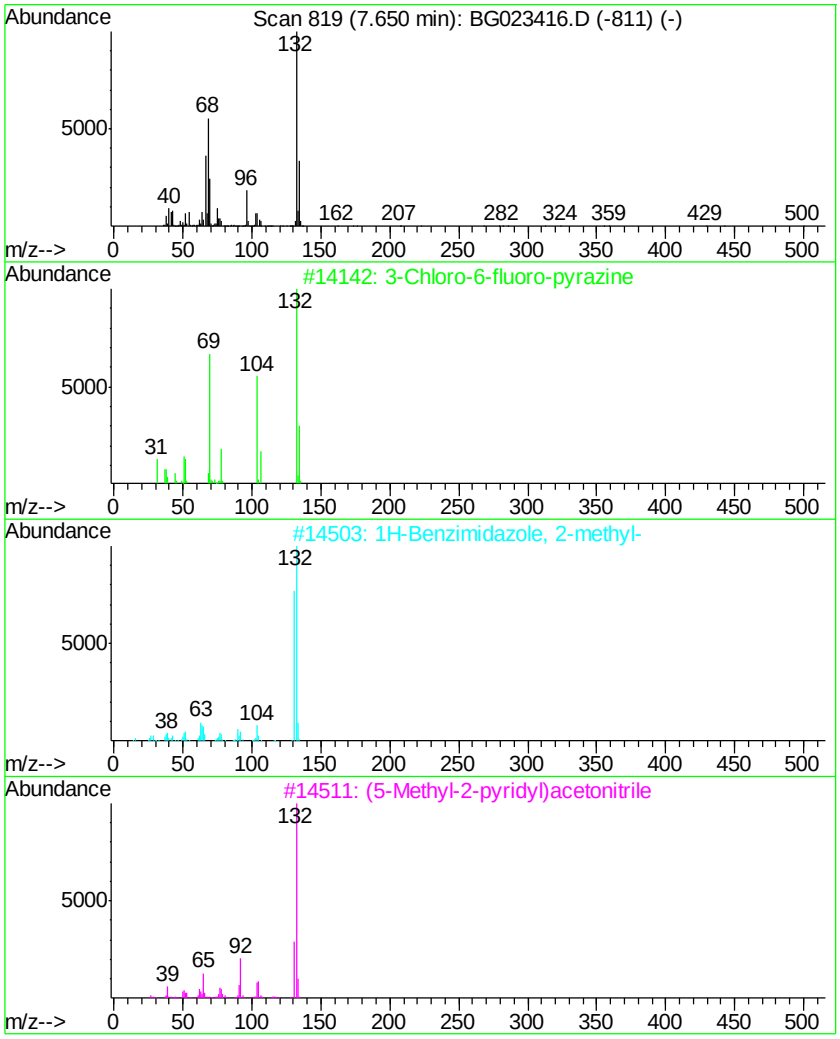
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

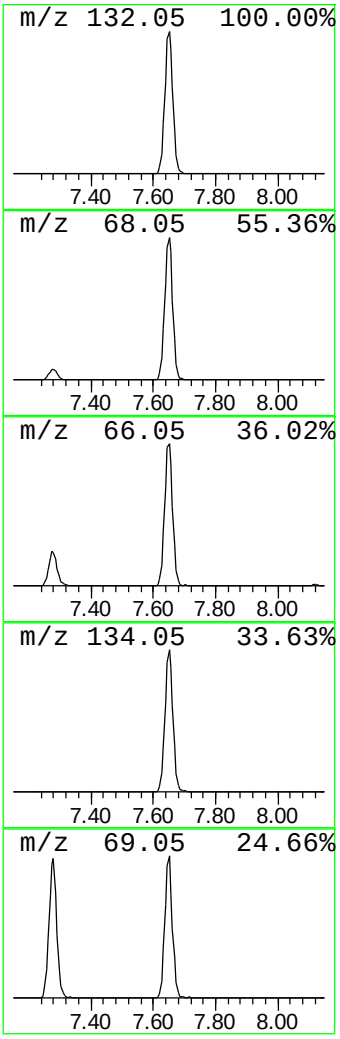
****

Peak Number 3 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	120.35 ng	4020510	1,4-Dichlorobenzene-d4	8.12

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-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14





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Operator : UM/SJ
Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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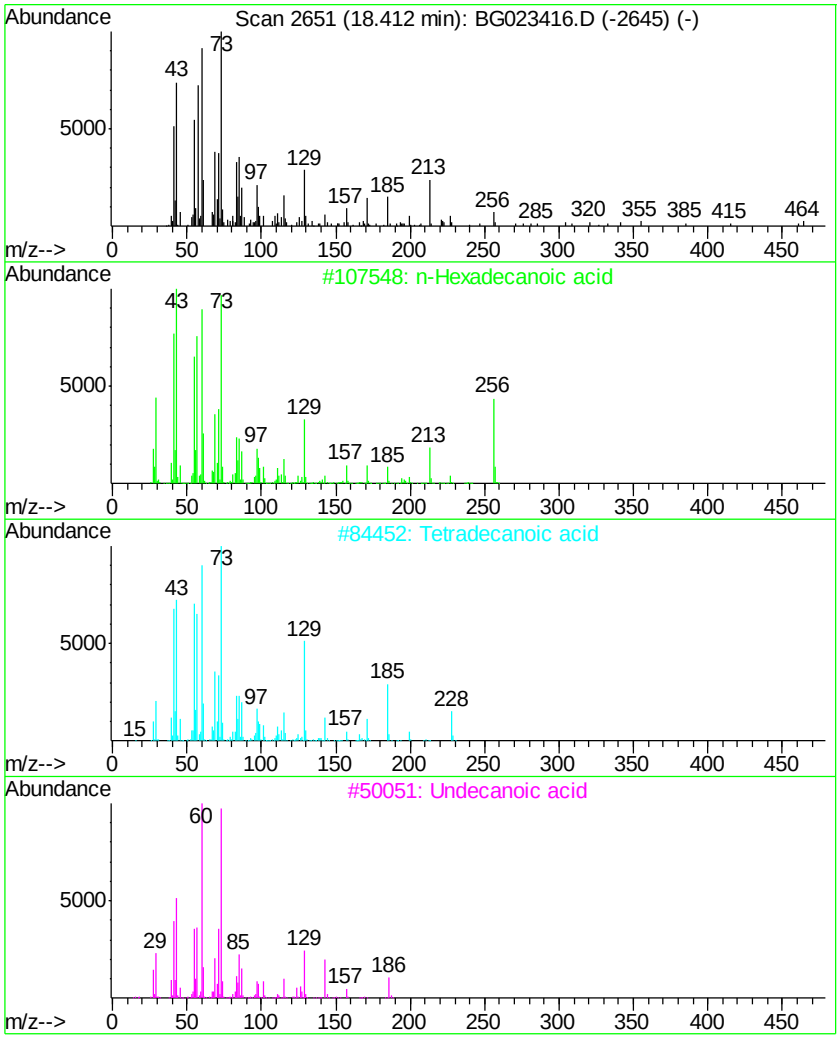
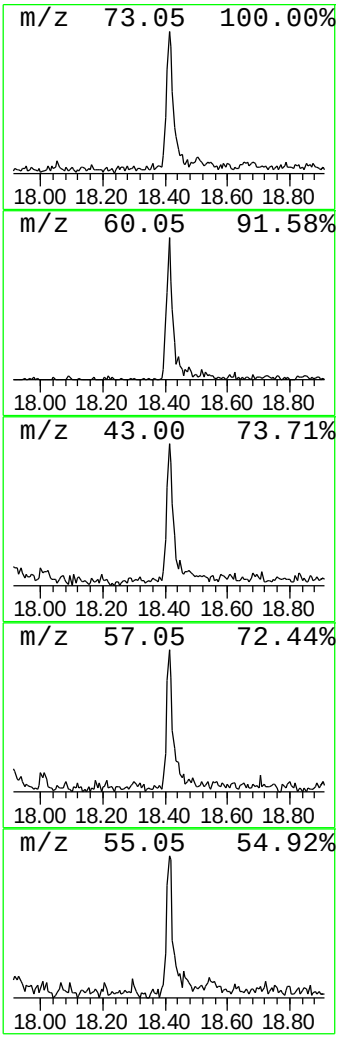
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.19 ng	277352	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3	Undecanoic acid	186	C11H22O2	000112-37-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	56





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Operator : UM/SJ
Sample : H4288-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-66-10.0-11.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
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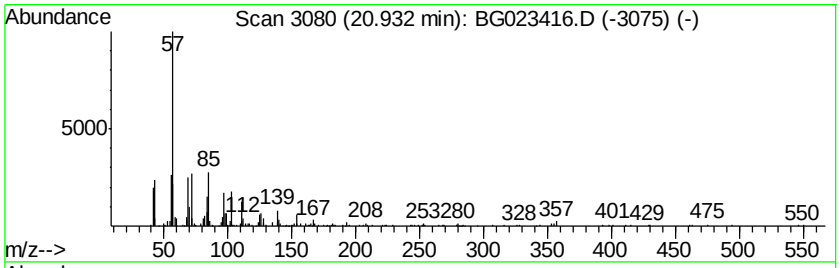
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

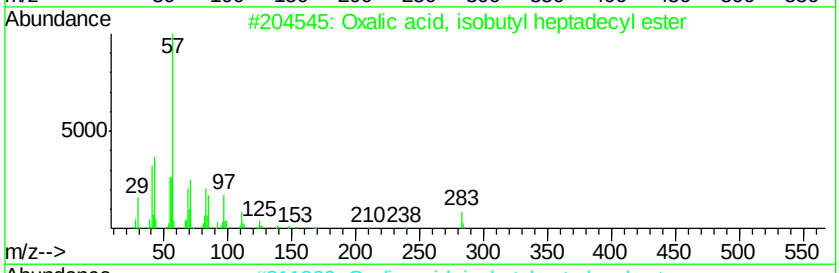
****

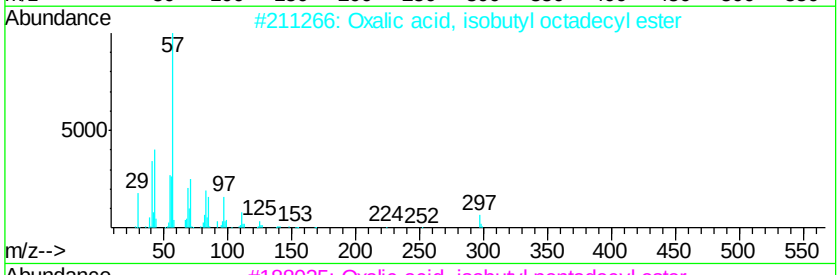
Peak Number 6 Oxalic acid, isobutyl hepta... Concentration Rank 6

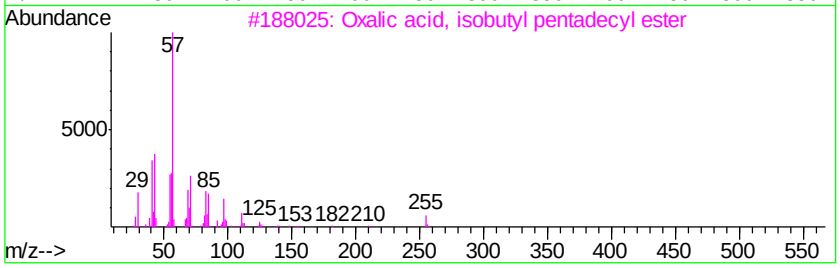
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	2.02 ng	242974	Chrysene-d12	21.85

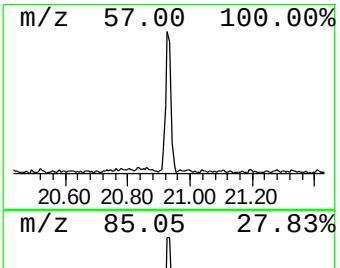
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	64
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	64
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	52
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	52
5	Isobutyl tridecyl carbonate	300	C18H36O3	959275-44-6	50

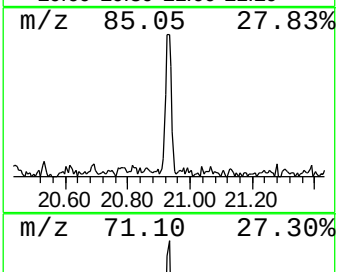


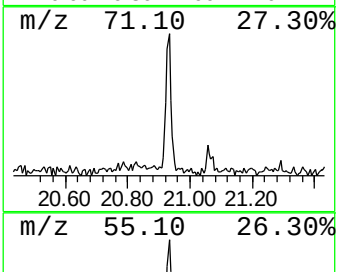


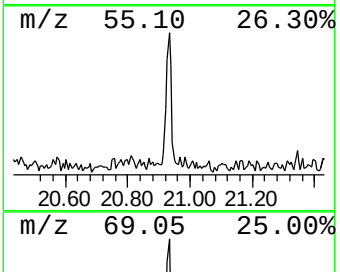


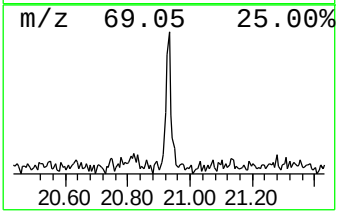












Tentatively Identified Compound (LSC) summary

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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
unknown2.99	2.99	254.0	ng	8486780	1	8.12	668137	20.0
2-Pentanone, 4-hy...	5.18	29.4	ng	982136	1	8.12	668137	20.0
unknown7.65	7.65	120.3	ng	4020510	1	8.12	668137	20.0
n-Hexadecanoic acid	18.41	2.2	ng	277352	4	17.54	2537170	20.0
Oxalic acid, isob...	20.93	2.0	ng	242974	5	21.85	2403810	20.0