LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG073116\
Data File : BG023363.D
Acq On : 30 Jul 2016 18:49
Operator : UM/SJ
Sample : H4223-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-36-2.5-3.5

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-BG072616.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	2.999	22	27	48	rBV	4994634	8457834	80.55%	10.546%
2	5.196	393	401	411	rBV	1102081	1783284	16.98%	2.224%
3	5.672	474	482	496	rBV	2796507	4791171	45.63%	5.974%
4	7.293	749	758	775	rBV	3272686	6139936	58.48%	7.656%
5	7.663	814	821	832	rBV	3178422	5543913	52.80%	6.913%
6	8.133	893	901	908	rBV	513894	898632	8.56%	1.120%
7	8.462	949	957	965	rBV	2166364	3837278	36.55%	4.785%
8	9.314	1092	1102	1112	rBV	2162045	3933399	37.46%	4.904%
9	10.971	1377	1384	1396	rBV	878970	1612930	15.36%	2.011%
10	13.420	1793	1801	1810	rBV	5832370	9516961	90.64%	11.866%
11	14.249	1935	1942	1949	rBV	1098370	1627587	15.50%	2.029%
12	14.677	2010	2015	2019	rVB	82392	116473	1.11%	0.145%
13	14.807	2030	2037	2046	rVB2	1662931	2668831	25.42%	3.328%
14	15.629	2172	2177	2182	rVB	192753	245393	2.34%	0.306%
15	16.305	2285	2292	2309	rVB	5471788	8818482	83.99%	10.995%
16	16.493	2320	2324	2335	rVB	197891	338926	3.23%	0.423%
17	17.291	2456	2460	2465	rBV2	104024	131201	1.25%	0.164%
18	17.568	2500	2507	2521	rBV	2105179	3303887	31.47%	4.120%
19	18.437	2650	2655	2661	rBV3	192604	358746	3.42%	0.447%
20	19.712	2868	2872	2879	rBV7	82830	160367	1.53%	0.200%
21	20.176	2945	2951	2957	rBV	7478598	10499511	100.00%	13.092%
22	21.885	3236	3242	3249	rBV2	1564607	2755135	26.24%	3.435%
23	25.287	3811	3821	3834	rBV3	888343	2660984	25.34%	3.318%

Sum of corrected areas: 80200861

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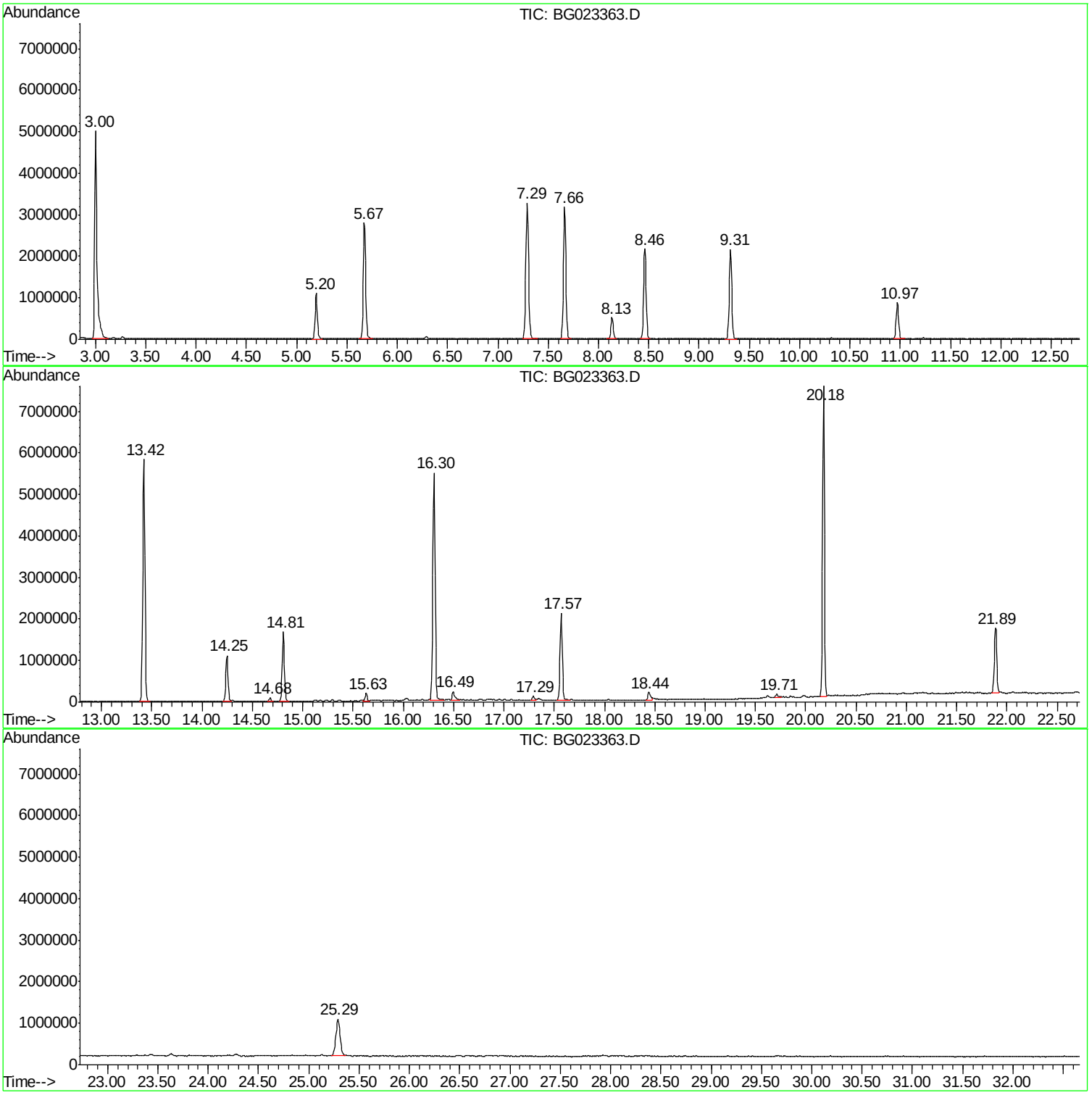
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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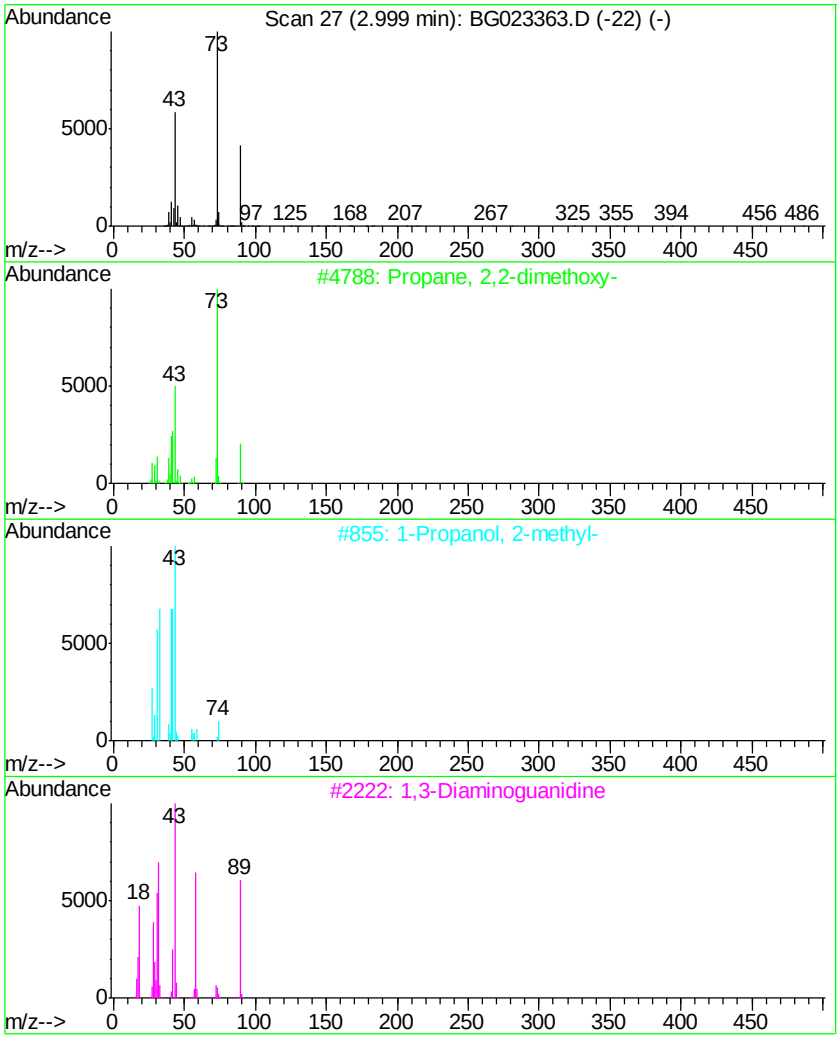
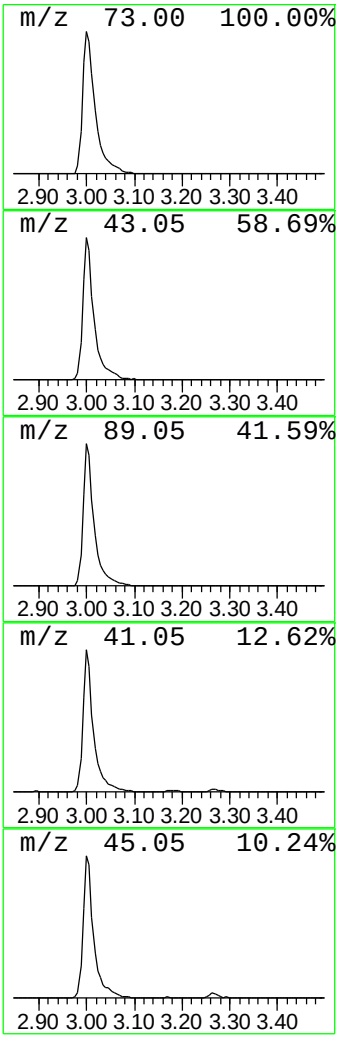
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	188.24 ng	8457830	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG073116\
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Misc :
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Instrument : BNA_G
ClientSampleId : SB-36-2.5-3.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.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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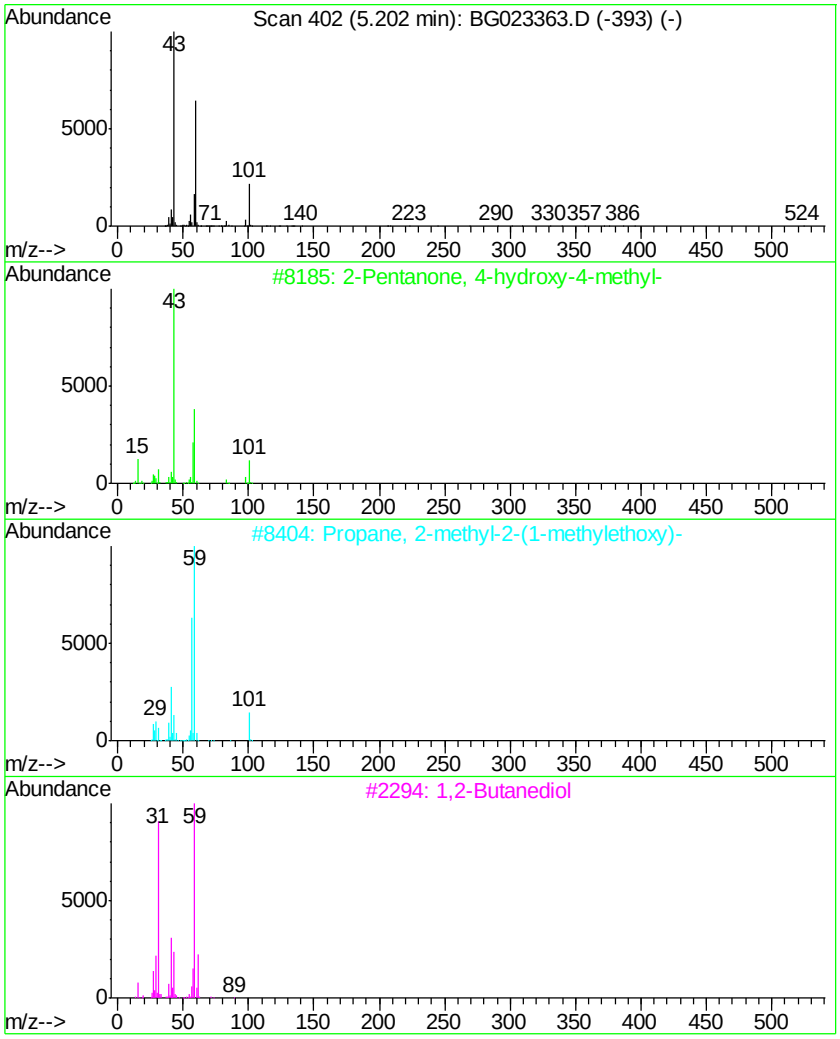
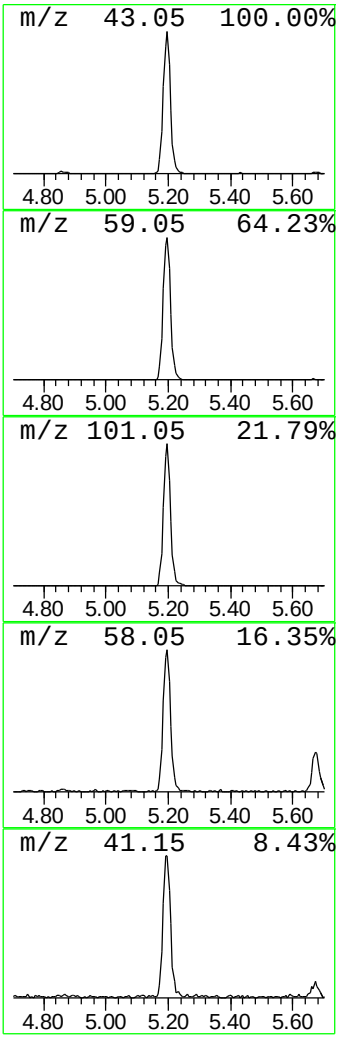
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	39.69 ng	1783280	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	1,2-Butanediol	90	C4H10O2	000584-03-2	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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ClientSampleId : SB-36-2.5-3.5

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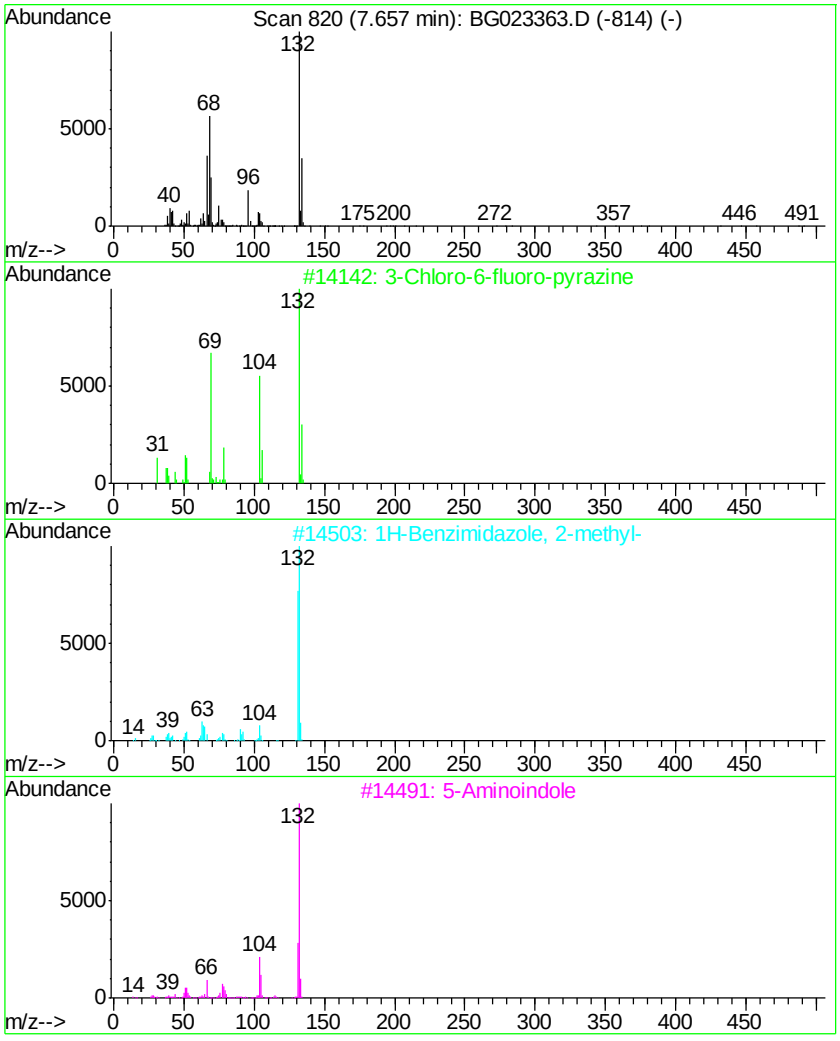
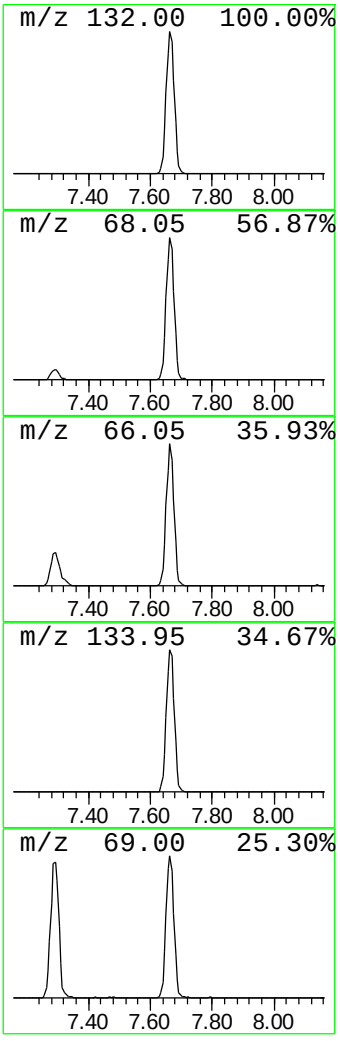
Peak Number 3 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	123.39 ng	5543910	1,4-Dichlorobenzene-d4	8.13

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Instrument : BNA_G
ClientSampleId : SB-36-2.5-3.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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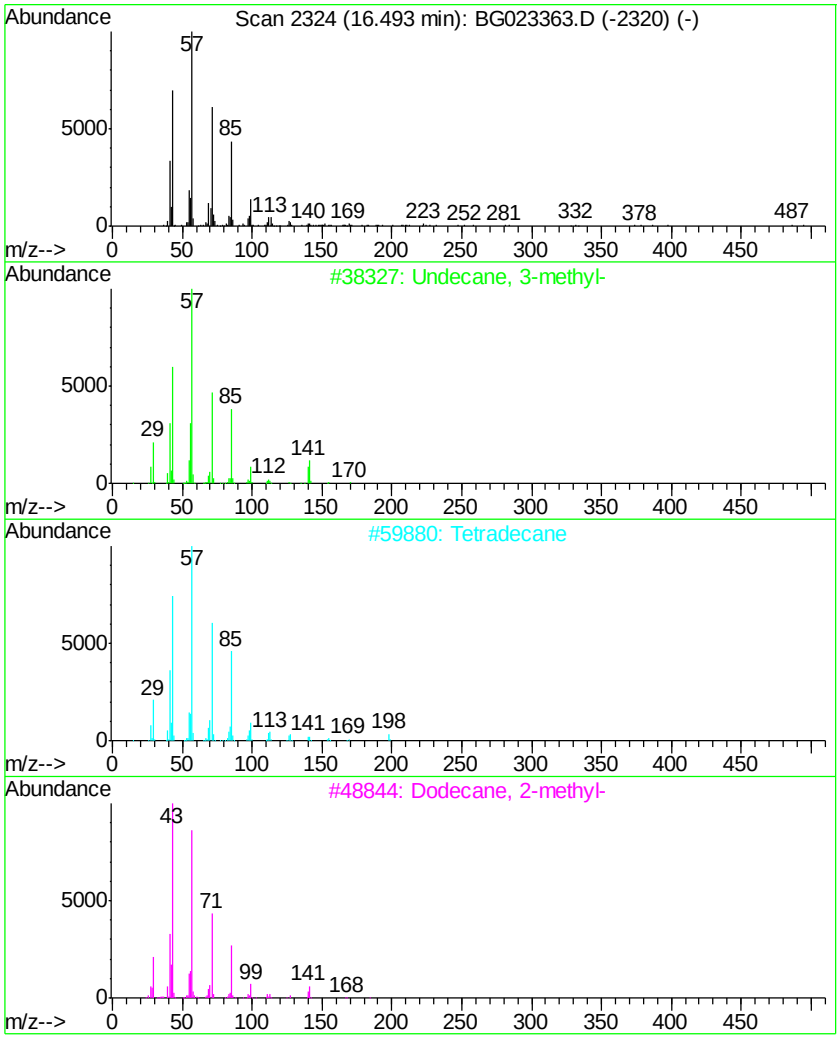
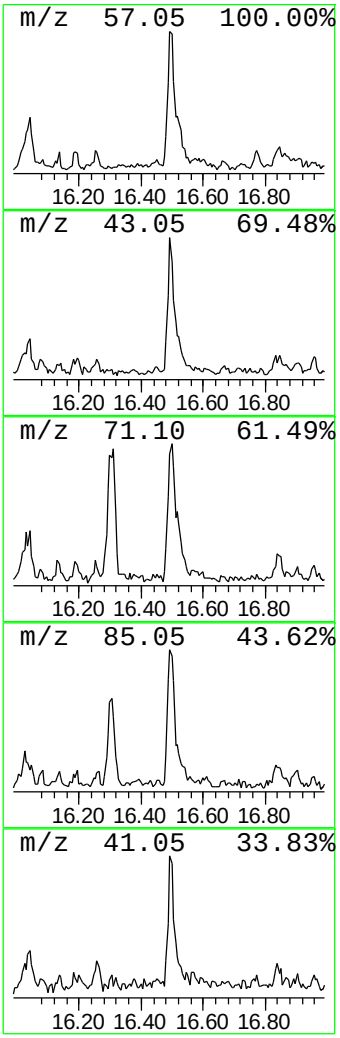
Peak Number 5 Undecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.05 ng	338926	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3-methyl-	170	C12H26	001002-43-3	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Heptadecane	240	C17H36	000629-78-7	78





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Instrument : BNA_G
ClientSampleId : SB-36-2.5-3.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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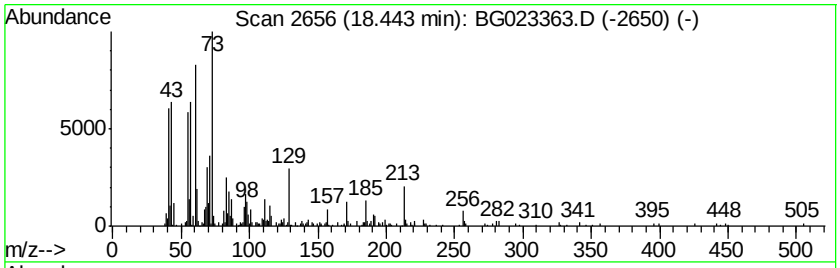
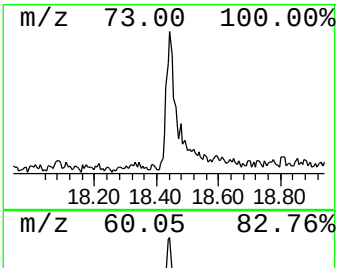
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	2.17 ng	358746	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	74
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	3.00	188.2	ng	8457830	1	8.13	898632	20.0
2-Pentanone, 4-hy...	5.20	39.7	ng	1783280	1	8.13	898632	20.0
unknown7.66	7.66	123.4	ng	5543910	1	8.13	898632	20.0
Undecane, 3-methyl-	16.49	2.0	ng	338926	4	17.57	3303890	20.0
n-Hexadecanoic acid	18.44	2.2	ng	358746	4	17.57	3303890	20.0