LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027398.D
Acq On : 13 Jun 2017 22:59
Operator : SJ/MA
Sample : I3614-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-8

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	5.692	333	341	350	rBV	188950	310724	6.30%	1.685%
2	6.132	408	416	425	rBV	279205	472275	9.58%	2.561%
3	7.678	669	679	688	rBV	181465	338152	6.86%	1.834%
4	8.077	736	747	760	rBV	496278	916020	18.57%	4.967%
5	8.541	820	826	835	rVB	163140	296931	6.02%	1.610%
6	8.870	874	882	891	rVB	622346	1167756	23.68%	6.332%
7	9.705	1016	1024	1038	rBV	568707	1088604	22.07%	5.903%
8	11.356	1297	1305	1313	rBV	242428	472800	9.59%	2.564%
9	12.584	1507	1514	1524	rVB2	25820	50847	1.03%	0.276%
10	13.747	1703	1712	1722	rVB	1582448	2603797	52.79%	14.120%
11	14.311	1801	1808	1815	rBV9	18608	51024	1.03%	0.277%
12	14.552	1843	1849	1855	rVB	148708	237035	4.81%	1.285%
13	15.122	1939	1946	1952	rBV2	361593	620280	12.58%	3.364%
14	15.562	2016	2021	2025	rBV5	27843	55034	1.12%	0.298%
15	15.709	2041	2046	2053	rBV6	30859	70930	1.44%	0.385%
16	16.602	2191	2198	2209	rVB	892864	1504112	30.50%	8.156%
17	17.872	2407	2414	2425	rVB2	498279	839040	17.01%	4.550%
18	18.706	2552	2556	2561	rBV	73114	113188	2.30%	0.614%
19	19.963	2766	2770	2780	rBV4	54771	98758	2.00%	0.536%
20	20.445	2846	2852	2863	rVB	3456356	4931914	100.00%	26.744%
21	21.362	3004	3008	3014	rVB	64118	96425	1.96%	0.523%
22	22.249	3152	3159	3169	rVB	573359	1082570	21.95%	5.870%
23	25.915	3772	3783	3795	rBV2	314462	1022840	20.74%	5.547%

Sum of corrected areas: 18441056

LSC Report - Integrated Chromatogram

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Operator : SJ/MA
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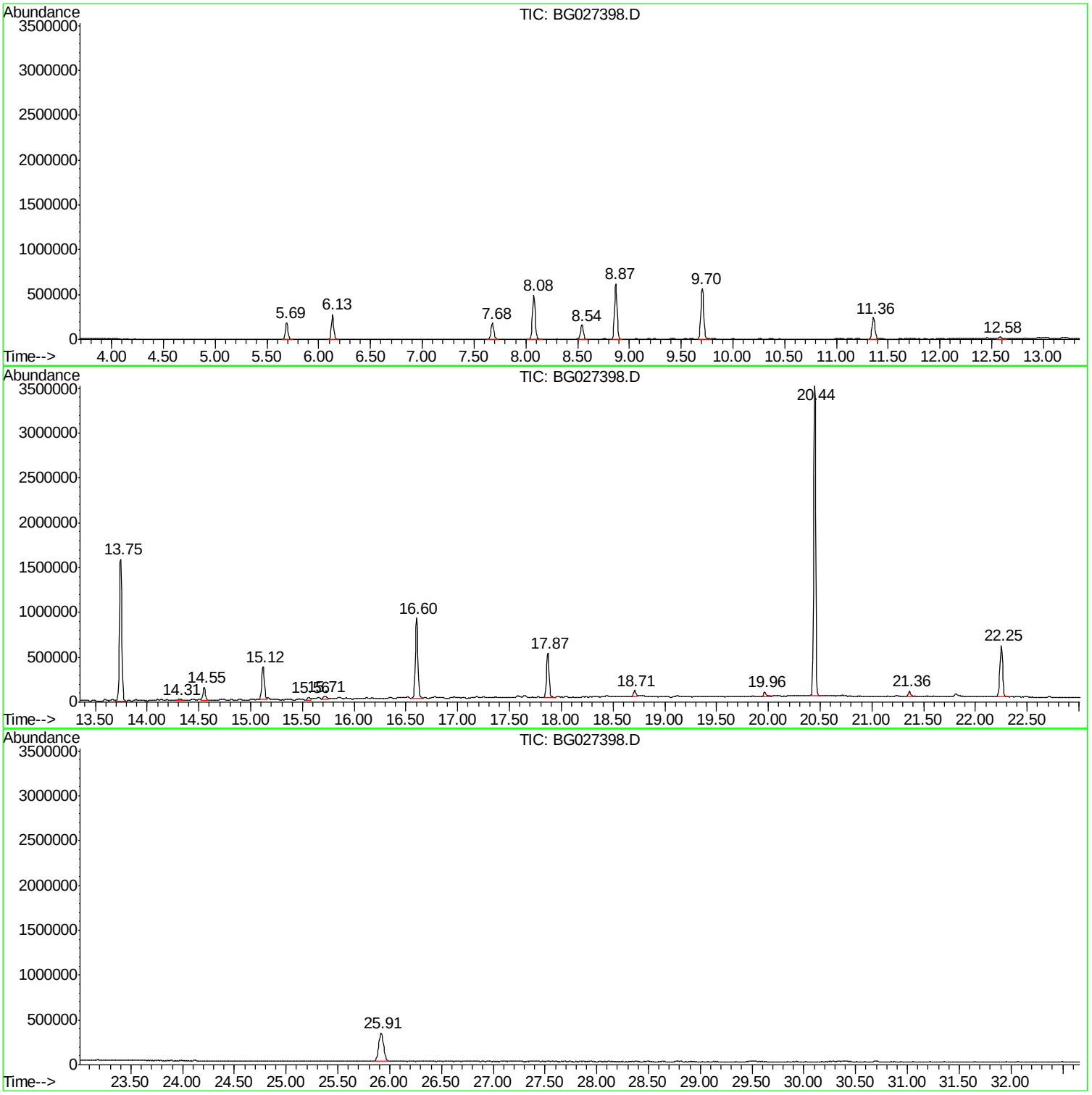
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-8

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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Data File : BG027398.D
Acq On : 13 Jun 2017 22:59
Operator : SJ/MA
Sample : I3614-08
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ClientSampleId : PZ-8

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

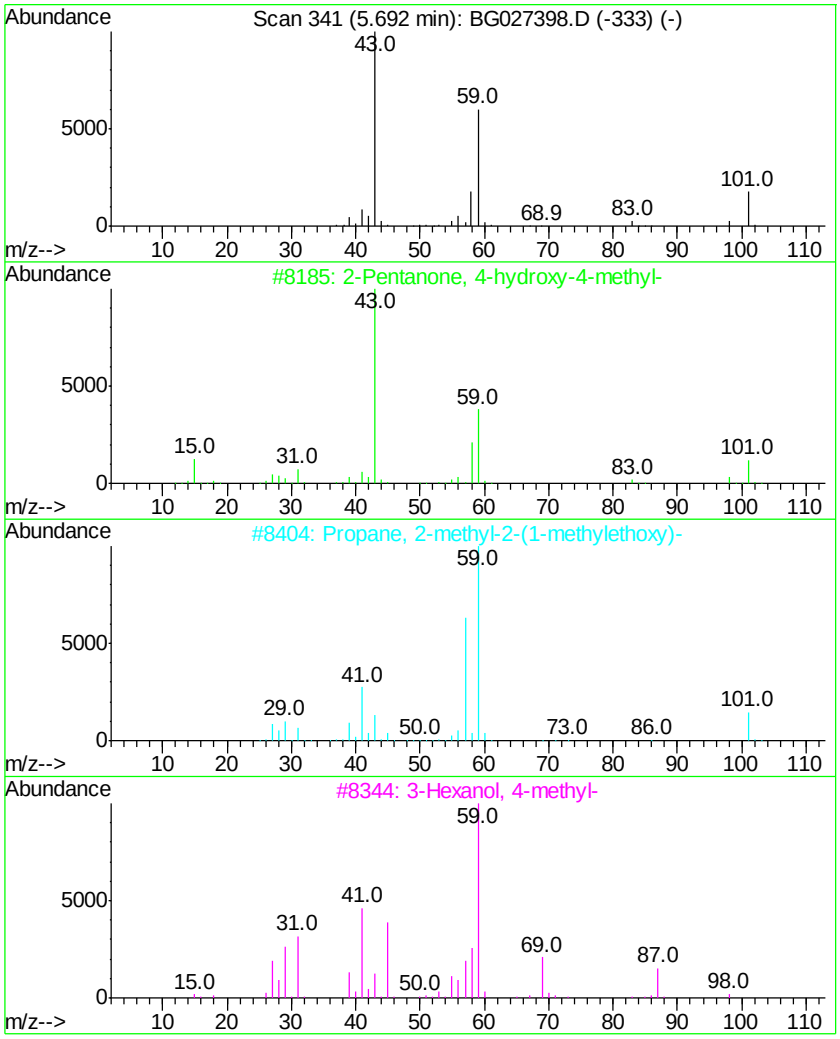
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

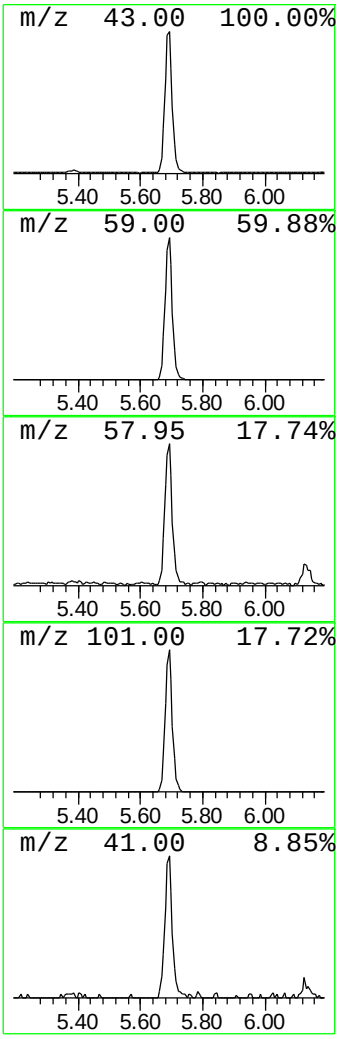
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	20.93 ng	310724	1,4-Dichlorobenzene-d4	8.54

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	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BG027398.D
Acq On : 13 Jun 2017 22:59
Operator : SJ/MA
Sample : I3614-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-8

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

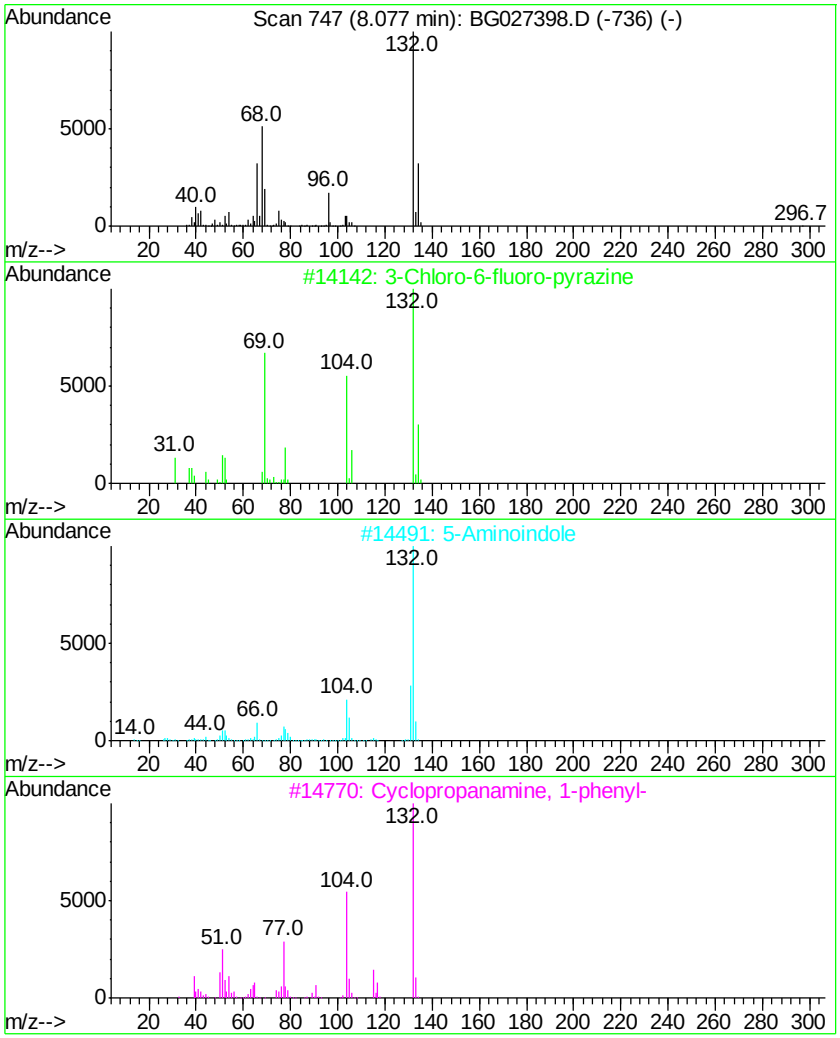
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

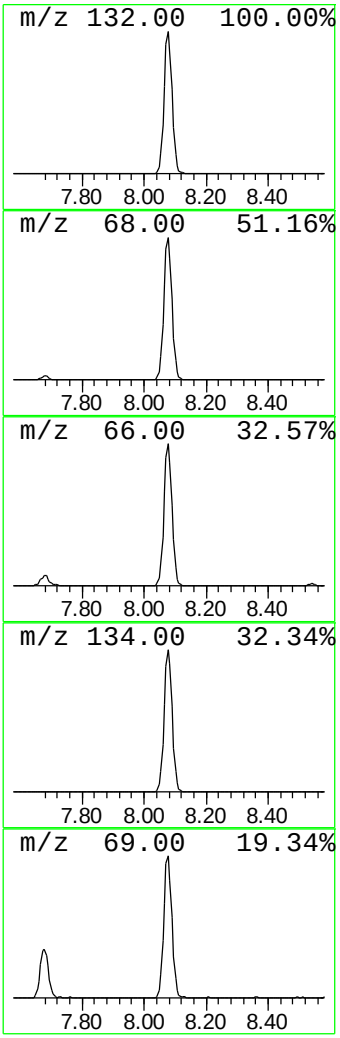
****

Peak Number 2 unknown8.08 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.08	61.70 ng	916020	1,4-Dichlorobenzene-d4	8.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Data File : BG027398.D
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Operator : SJ/MA
Sample : I3614-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-8

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
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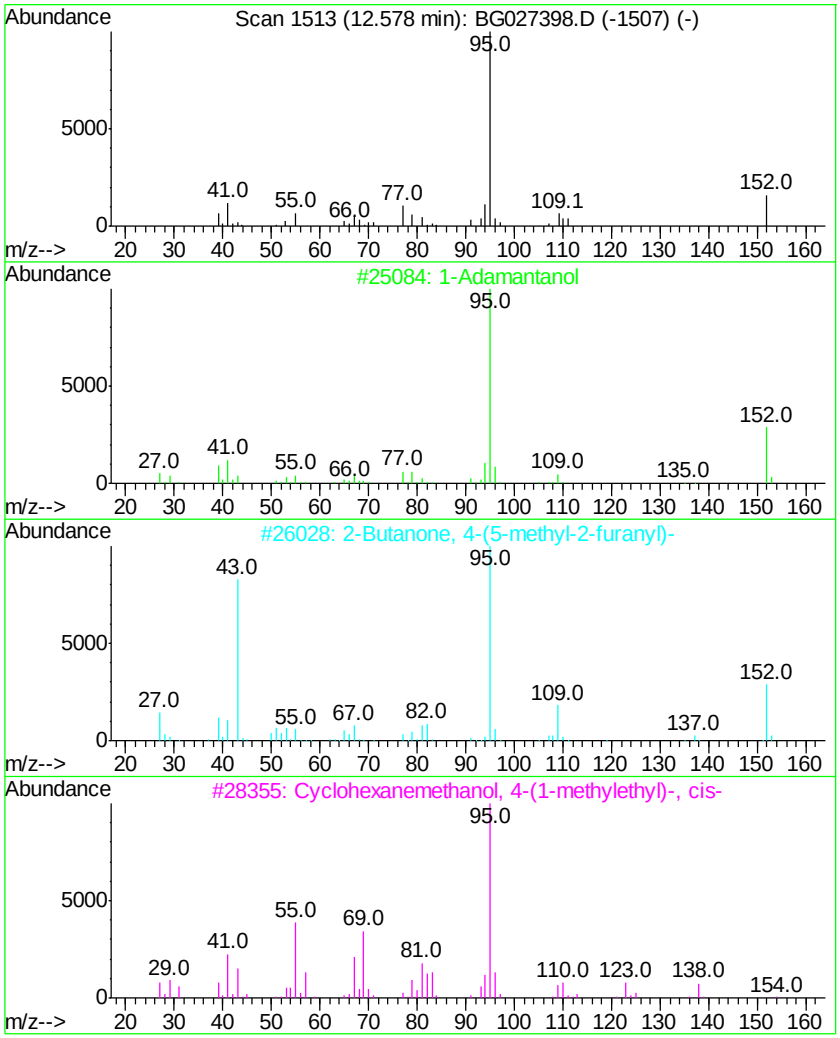
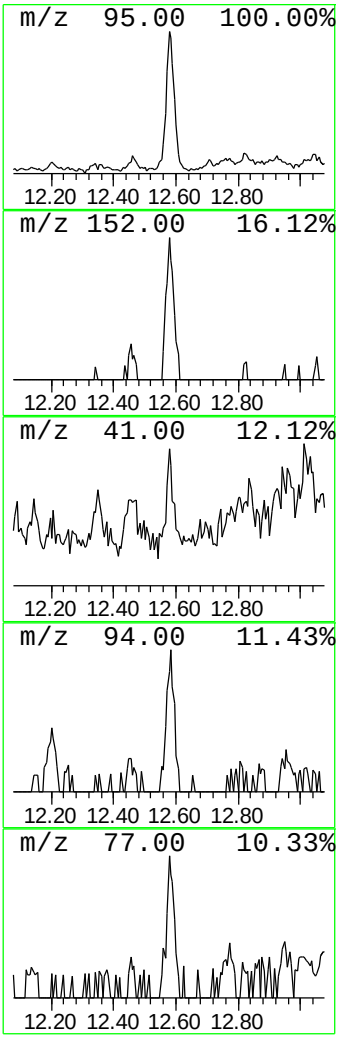
Peak Number 4 1-Adamantanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	2.15 ng	50847	Naphthalene-d8	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanol	152	C10H16O	000768-95-6	90
2	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	64
3	Cyclohexanemethanol, 4-(1-methyl...	156	C10H20O	013828-37-0	59
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	59
5	exo-2-Bromonorbornane	174	C7H11Br	002534-77-2	53





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Instrument : BNA_G
ClientSampleId : PZ-8

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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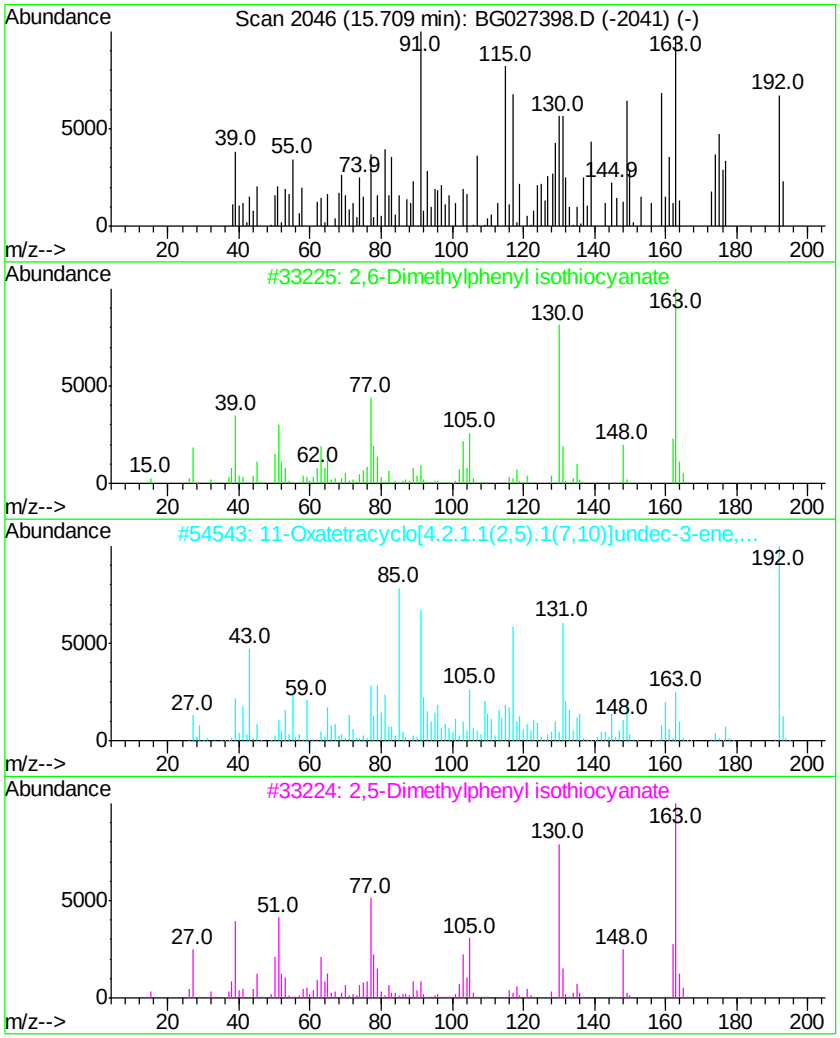
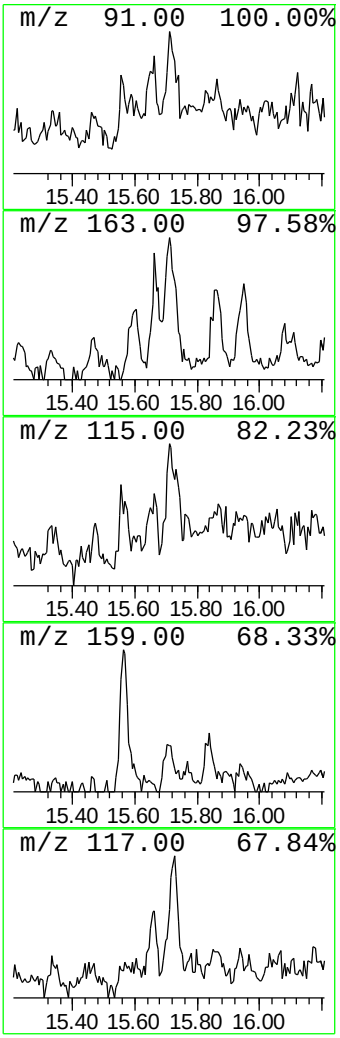
Peak Number 5 unknown15.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.29 ng	70930	Acenaphthene-d10	15.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethylphenyl isothiocyanate	163	C9H9NS	019241-16-8	18
2	11-Oxatetracyclo[4.2.1.1(2,5).1(...	192	C12H16O2	1000194-37-0	18
3	2,5-Dimethylphenyl isothiocyanate	163	C9H9NS	019241-15-7	18
4	5-Amino-2,2-dimethyl-2,3-dihydro...	163	C10H13NO	031010-94-3	15
5	2(1H)-Quinolinone, 1-methyl-	159	C10H9NO	000606-43-9	15





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Instrument : BNA_G
ClientSampleId : PZ-8

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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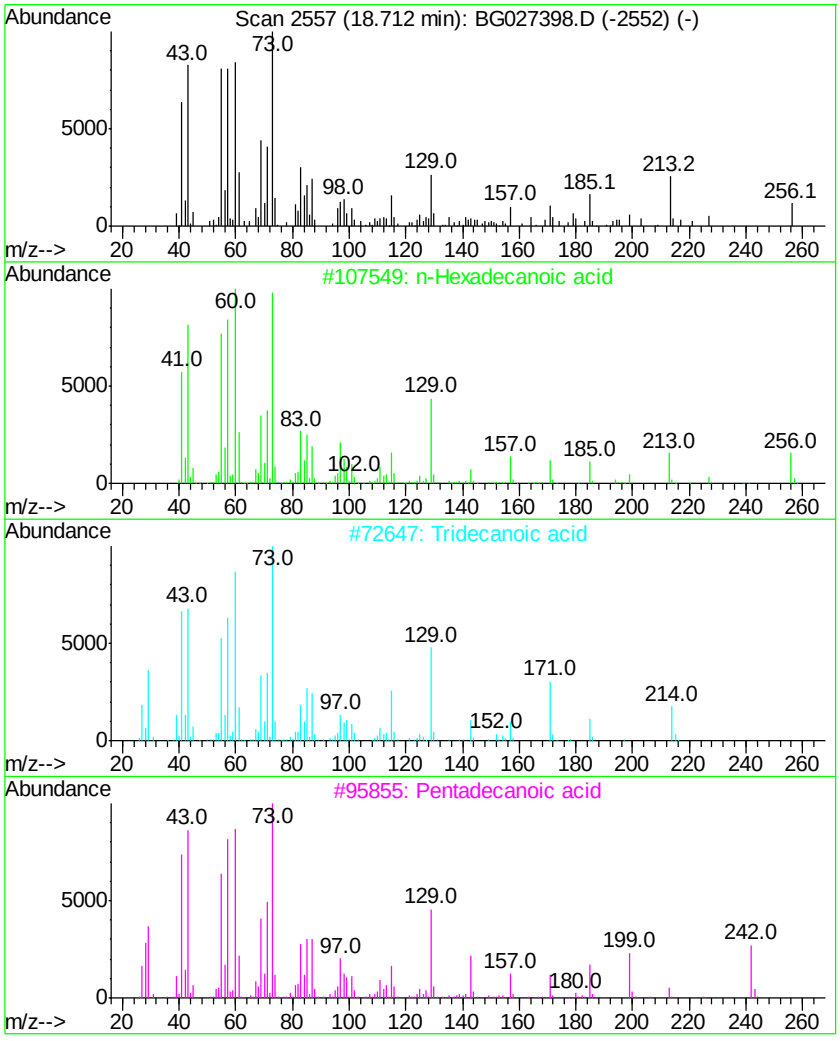
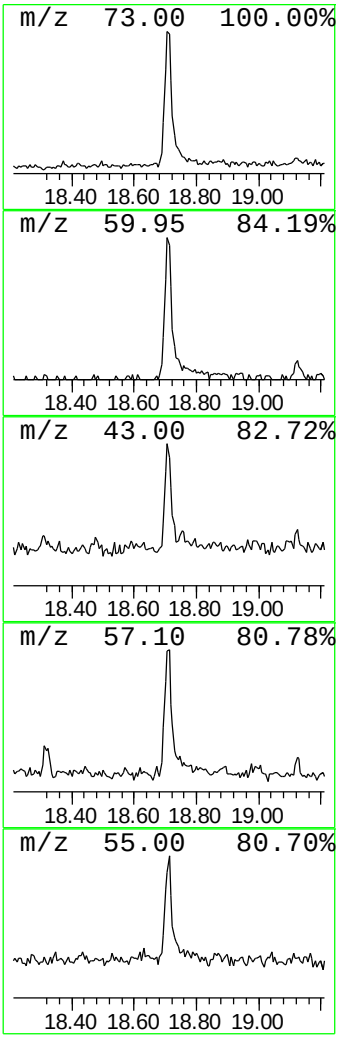
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.71	2.70 ng	113188	Phenanthrene-d10	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Isoamyl nitrite	117	C5H11NO2	000110-46-3	35





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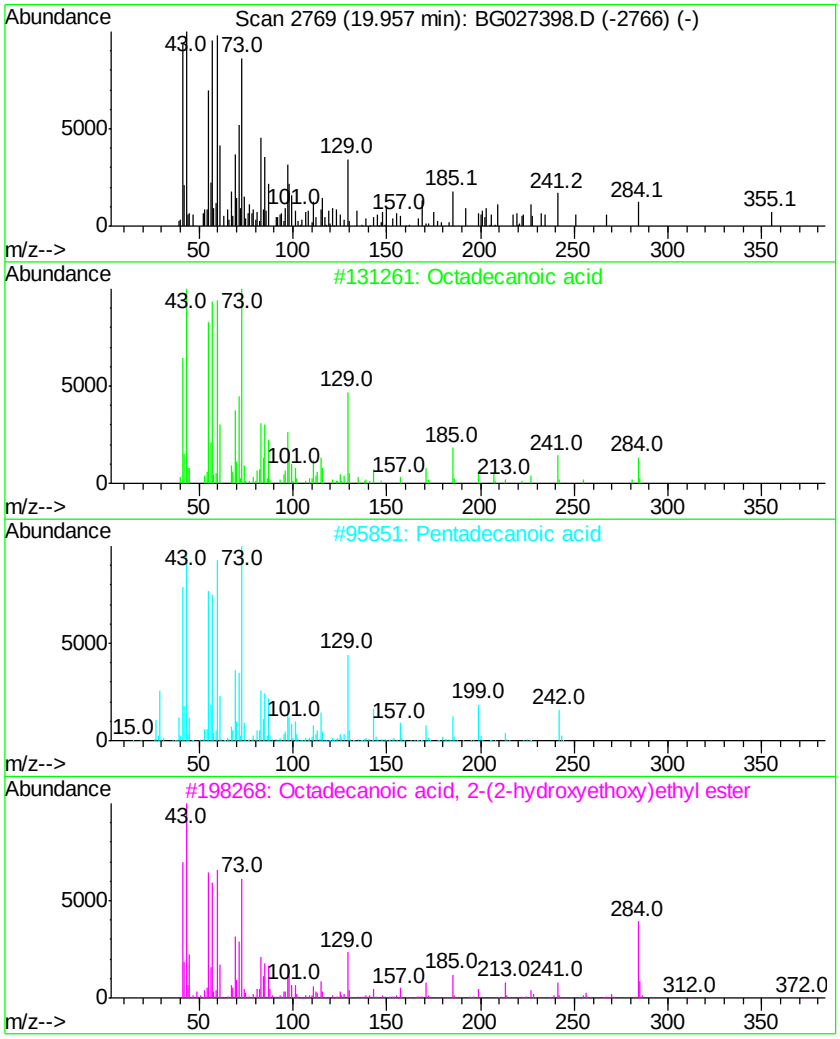
TIC Integration Parameters: LSCINT.P

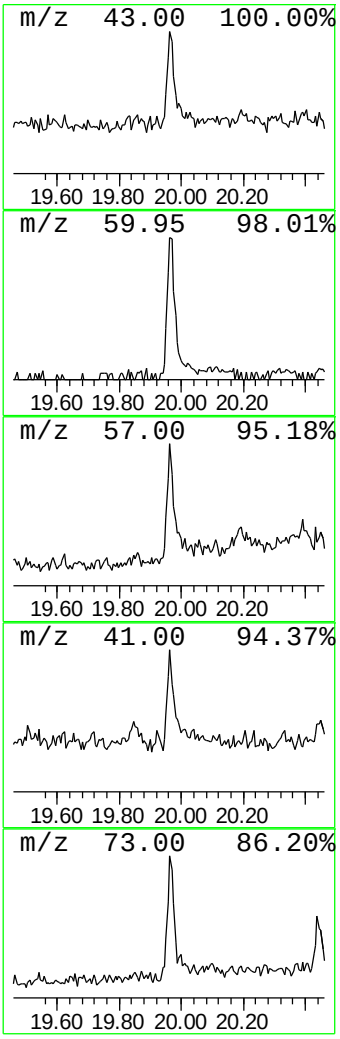
****

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.96	2.35 ng	98758	Phenanthrene-d10	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





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
2-Pentanone, 4-hy...	5.69	20.9	ng	310724	1	8.54	296931	20.0
unknown8.08	8.08	61.7	ng	916020	1	8.54	296931	20.0
1-Adamantanol	12.58	2.1	ng	50847	2	11.36	472800	20.0
unknown15.71	15.71	2.3	ng	70930	3	15.12	620280	20.0
n-Hexadecanoic acid	18.71	2.7	ng	113188	4	17.87	839040	20.0
Octadecanoic acid	19.96	2.4	ng	98758	4	17.87	839040	20.0