LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062818\
Data File : BG035500.D
Acq On : 29 Jun 2018 5:22
Operator : JU/SJ
Sample : J3718-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	5.162	314	319	327	rBV2	27463	41983	1.24%	0.288%
2	5.379	348	356	364	rVB	28381	48544	1.43%	0.333%
3	5.626	392	398	410	rVB	309917	505053	14.86%	3.467%
4	7.212	659	668	679	rBV	194848	359406	10.58%	2.467%
5	7.582	723	731	739	rBV	584451	1037324	30.52%	7.121%
6	8.052	802	811	819	rBV	125631	220189	6.48%	1.512%
7	8.375	858	866	875	rBV	558206	979824	28.83%	6.727%
8	9.215	1001	1009	1019	rBV	465943	856072	25.19%	5.877%
9	10.854	1282	1288	1297	rVB2	150498	276908	8.15%	1.901%
10	13.298	1694	1704	1711	rBV	1404953	2133657	62.78%	14.648%
11	13.738	1774	1779	1786	rBV2	22266	34941	1.03%	0.240%
12	14.120	1838	1844	1848	rBV	26413	43352	1.28%	0.298%
13	14.672	1930	1938	1947	rVB2	265029	425649	12.52%	2.922%
14	16.158	2184	2191	2199	rBV	1164698	1778715	52.34%	12.211%
15	16.399	2228	2232	2240	rVB2	21133	36981	1.09%	0.254%
16	16.493	2243	2248	2253	rBV	36168	58110	1.71%	0.399%
17	16.552	2253	2258	2264	rVV2	39584	76440	2.25%	0.525%
18	16.617	2264	2269	2272	rVV2	38749	53520	1.57%	0.367%
19	16.810	2297	2302	2310	rVB4	50953	102166	3.01%	0.701%
20	16.881	2310	2314	2323	rBV	47914	89243	2.63%	0.613%
21	16.951	2323	2326	2333	rVB2	30693	46594	1.37%	0.320%
22	17.416	2399	2405	2411	rBV	357074	564753	16.62%	3.877%
23	18.297	2551	2555	2563	rBV4	58553	90491	2.66%	0.621%
24	20.024	2843	2849	2859	rBV	2443071	3398541	100.00%	23.331%
25	21.334	3067	3072	3075	rBV7	25347	48394	1.42%	0.332%
26	21.680	3125	3131	3139	rBV2	391584	657356	19.34%	4.513%
27	24.900	3669	3679	3691	rBV2	202223	602272	17.72%	4.135%

Sum of corrected areas: 14566478

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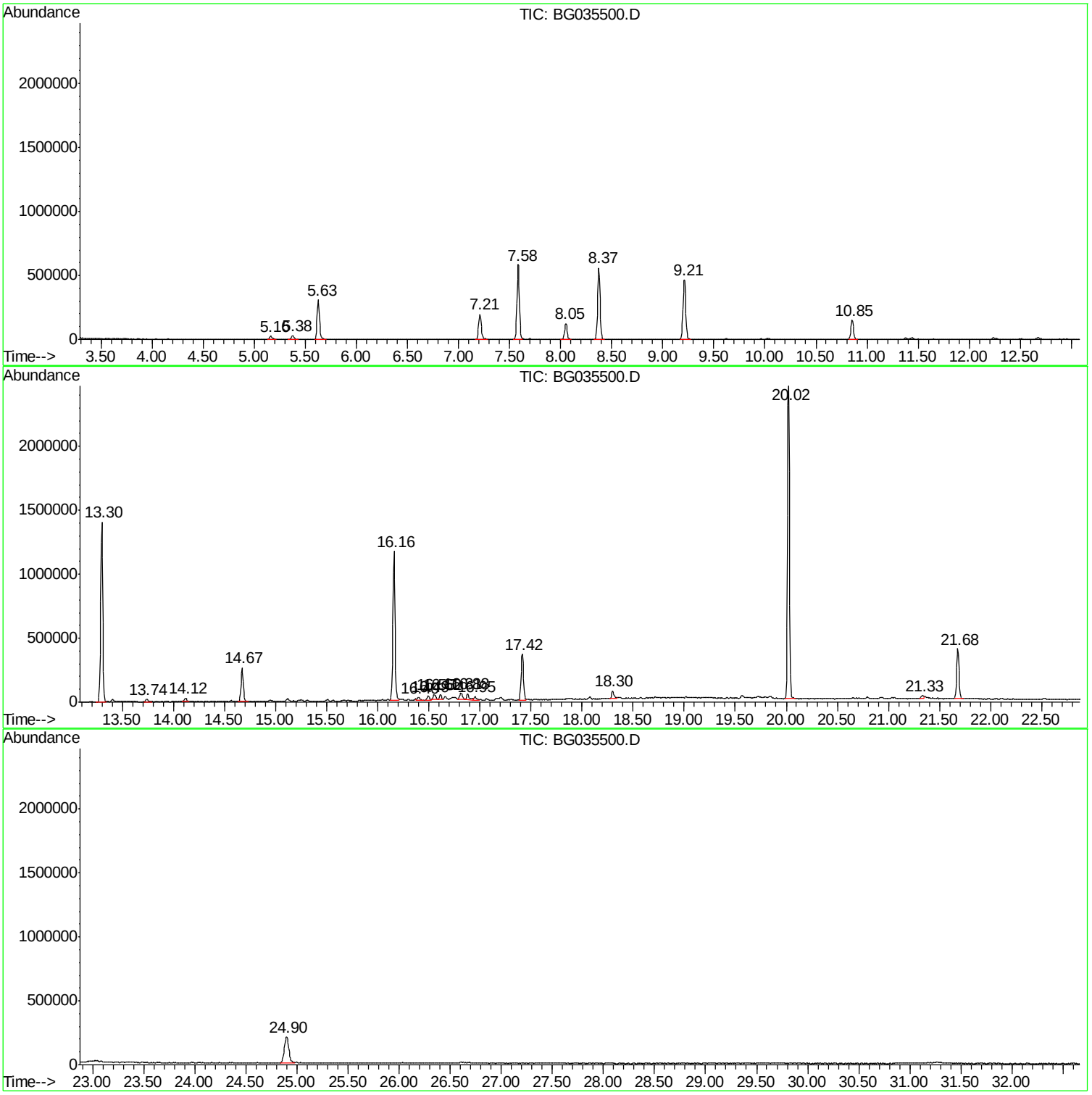
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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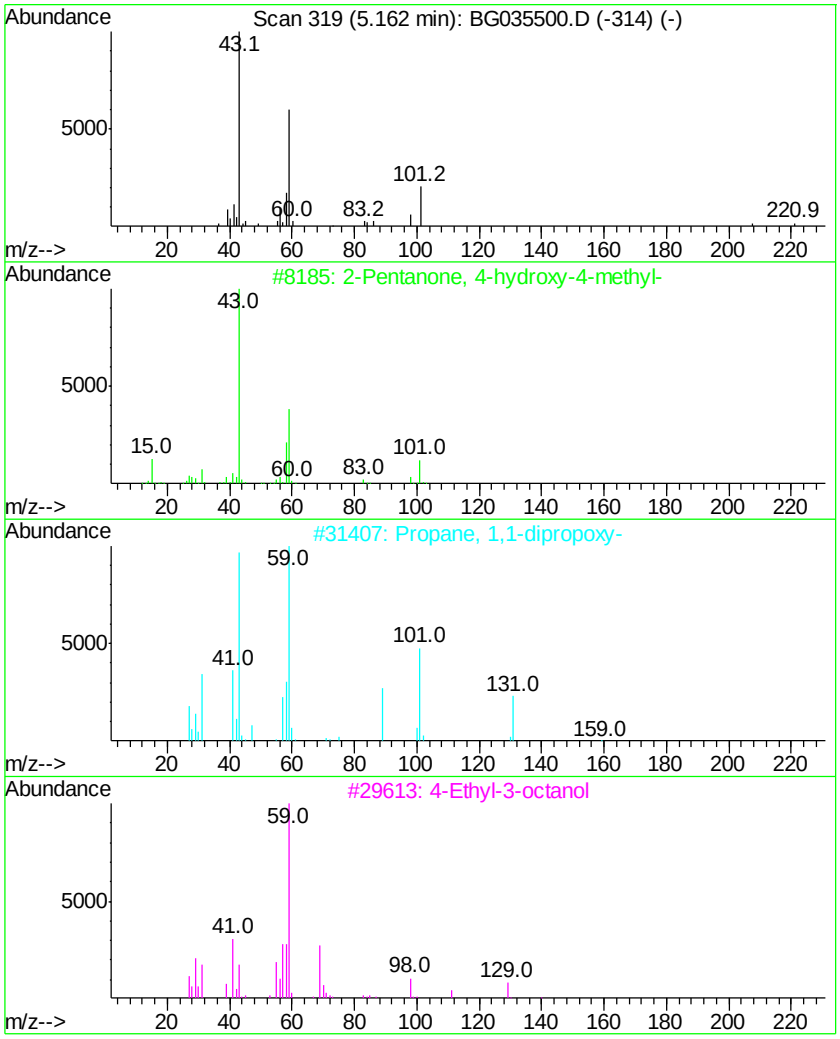
TIC Integration Parameters: LSCINT.P

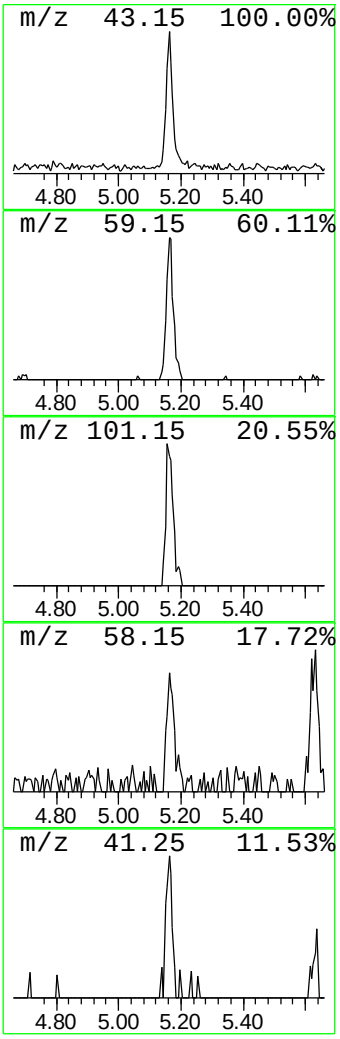
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.81 ng	41983	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36
3	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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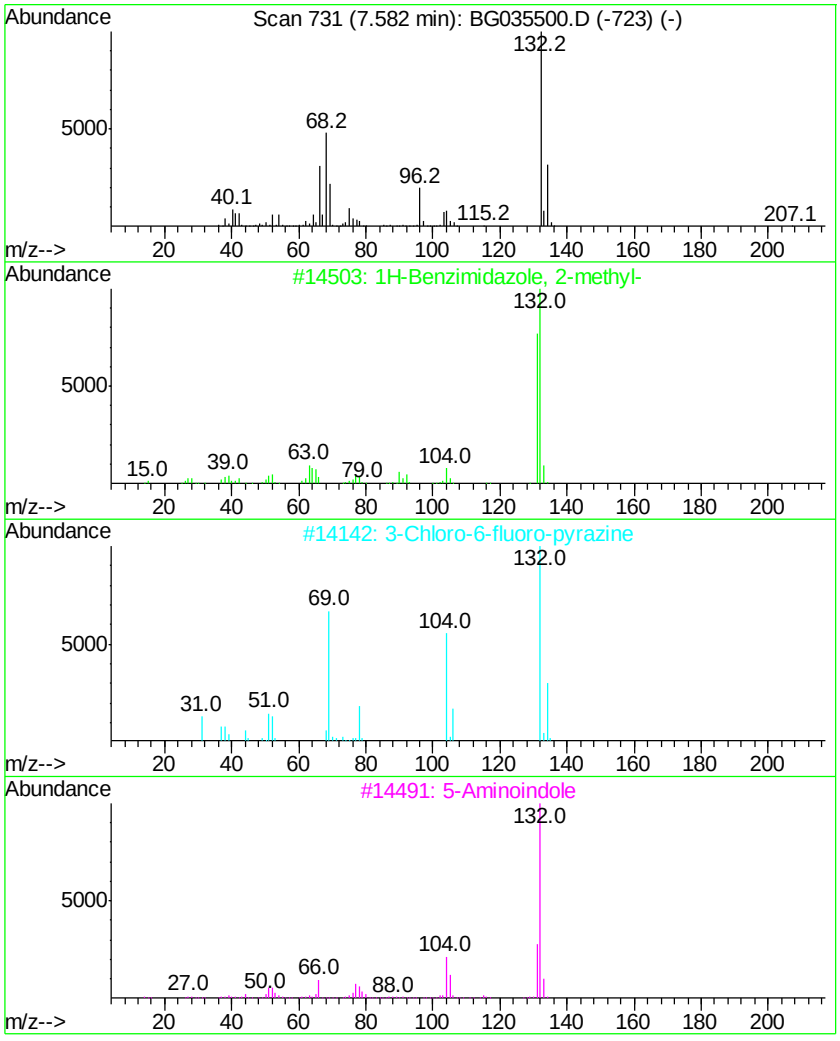
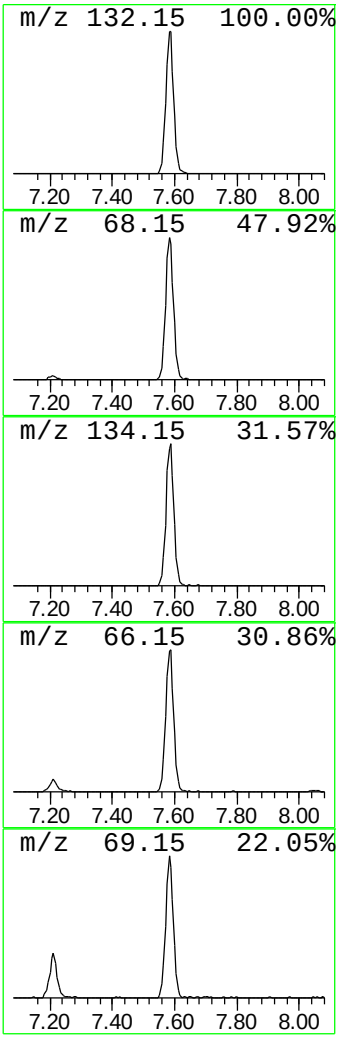
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	94.22 ng	1037320	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Operator : JU/SJ
Sample : J3718-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

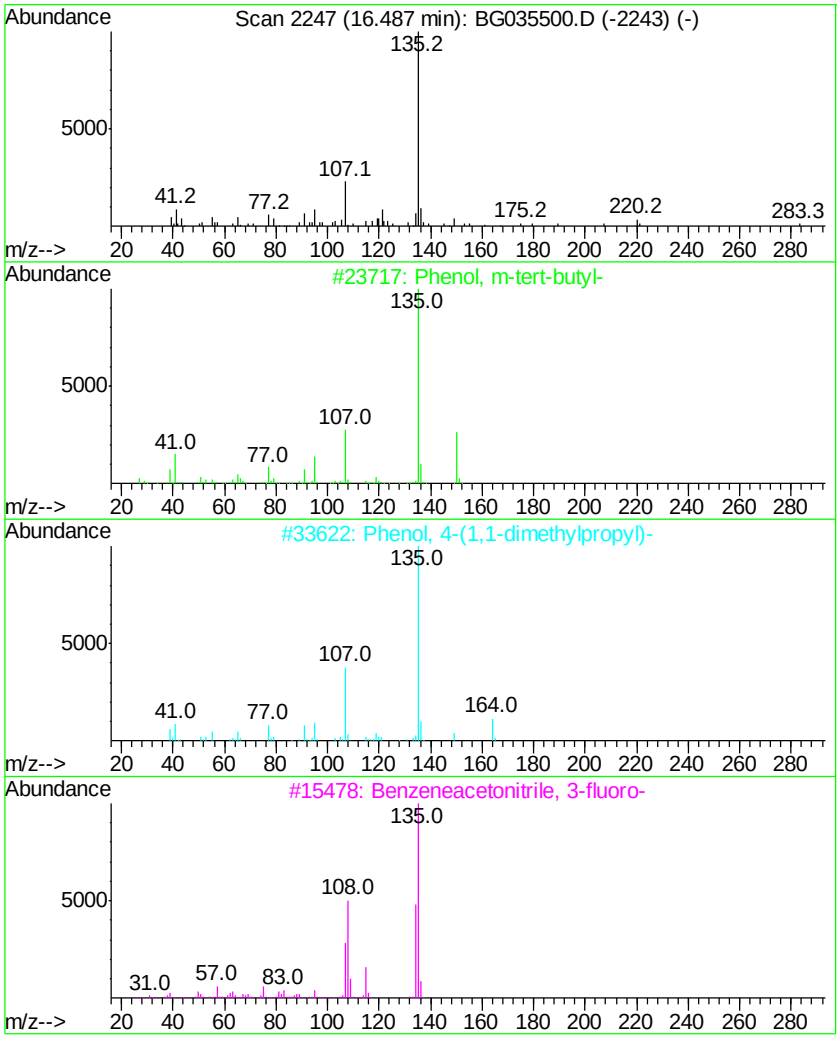
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

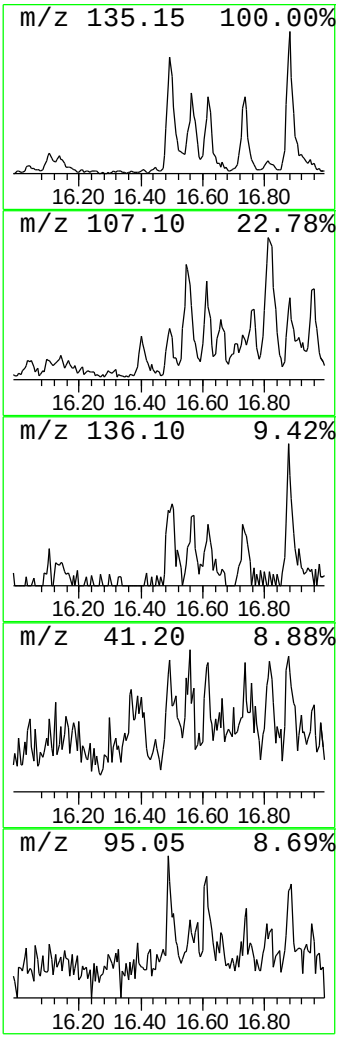
****

Peak Number 5 Phenol, m-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.06 ng	58110	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
3	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	64
4	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062818\
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Operator : JU/SJ
Sample : J3718-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

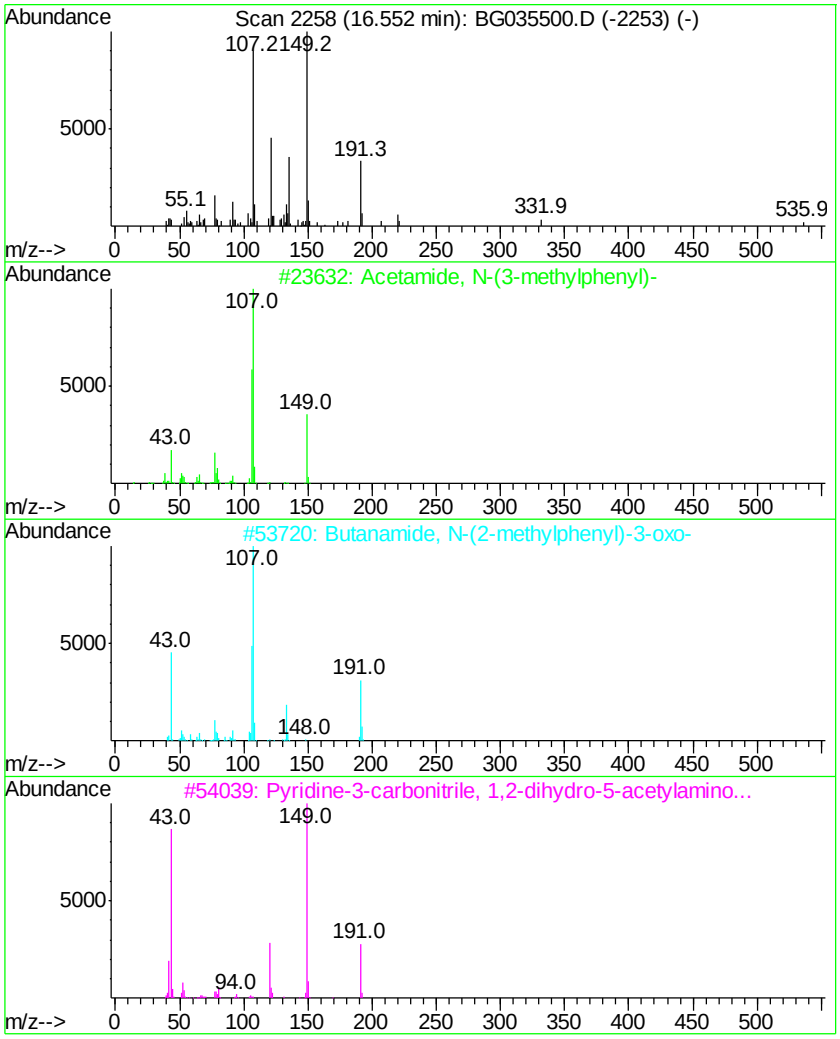
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

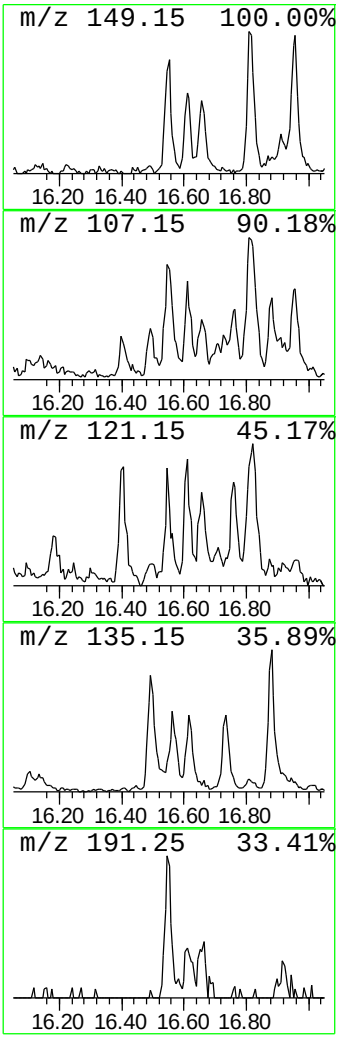
****

Peak Number 6 Acetamide, N-(3-methylphenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.71 ng	76440	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	58
2	Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	35
3	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	35
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	35
5	1,2-propanedione,1-(3,4-methylen...	192	C10H8O4	1000378-93-0	30





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

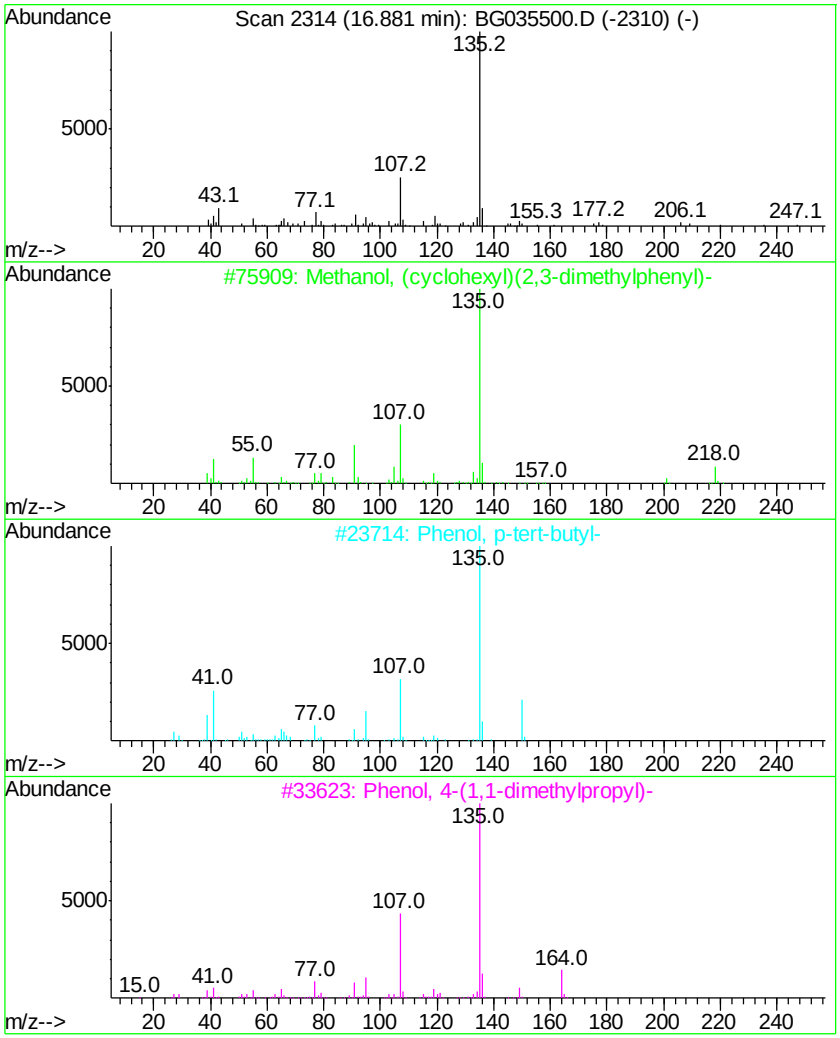
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

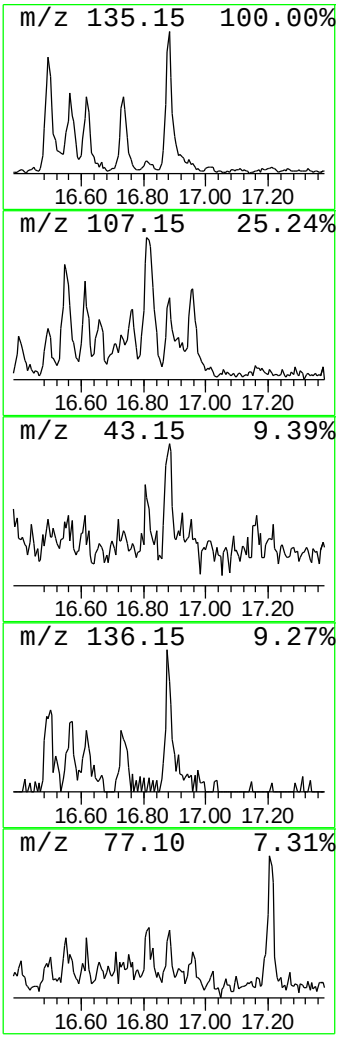
****

Peak Number 8 Methanol, (cyclohexyl)(2,3-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	3.16 ng	89243	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanol, (cyclohexyl)(2,3-dimet...	218	C15H22O	349498-47-1	72
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64
4	Adenine	135	C5H5N5	000073-24-5	59
5	1-Dodecanone, 2-(imidazol-1-yl)-...	356	C22H32N2O2	1000137-95-7	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062818\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

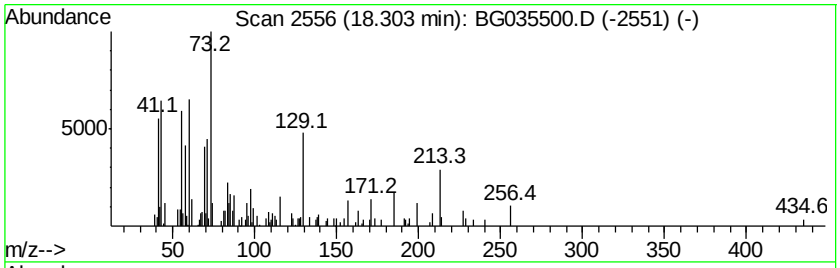
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

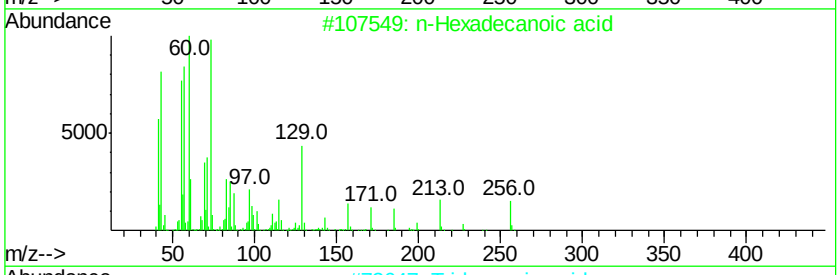
****

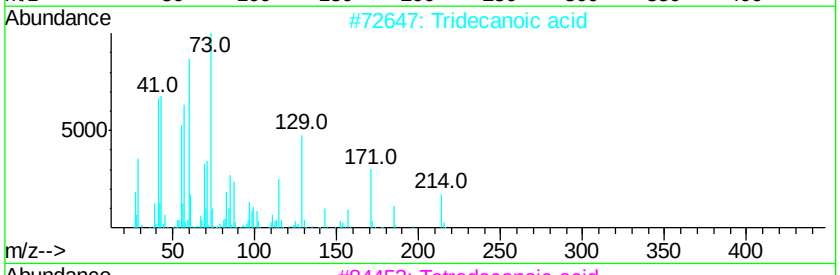
Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

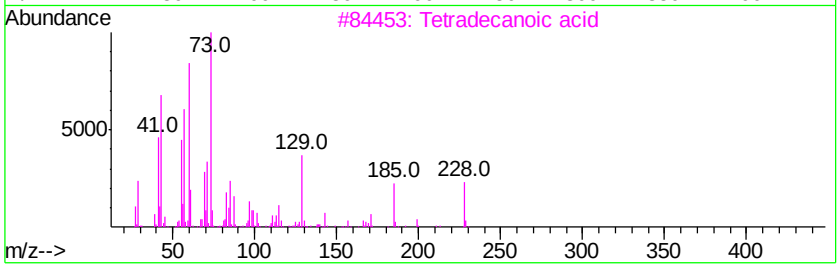
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.20 ng	90491	Phenanthrene-d10	17.42

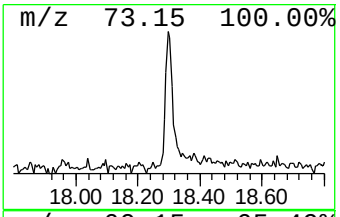
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64

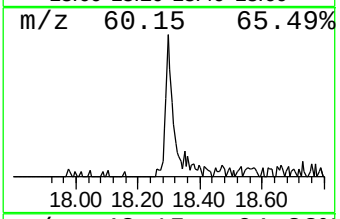


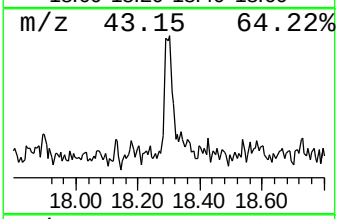


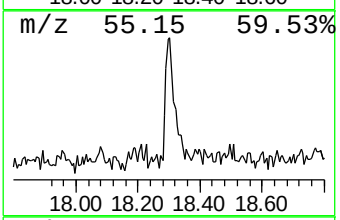


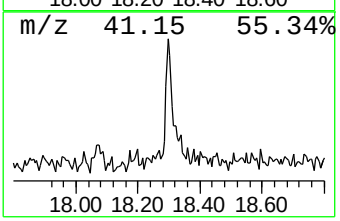












Tentatively Identified Compound (LSC) summary

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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...	5.16	3.8	ng	41983	1	8.05	220189	20.0
unknown7.58	7.58	94.2	ng	1037320	1	8.05	220189	20.0
Phenol, m-tert-bu...	16.49	2.1	ng	58110	4	17.42	564753	20.0
Acetamide, N-(3-m...	16.55	2.7	ng	76440	4	17.42	564753	20.0
Methanol, (cycloh...	16.88	3.2	ng	89243	4	17.42	564753	20.0
n-Hexadecanoic acid	18.30	3.2	ng	90491	4	17.42	564753	20.0