LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038514.D
Acq On : 13 Dec 2018 1:20
Operator : JU/SJ
Sample : J6331-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

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-BG121218.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	3.182	12	16	25	rVB	54402	88466	3.75%	0.855%
2	3.735	106	110	118	rBV	16934	28153	1.19%	0.272%
3	5.139	344	349	355	rBV	28566	44726	1.89%	0.432%
4	5.603	422	428	439	rBV	425383	722708	30.62%	6.988%
5	7.213	694	702	715	rBV	457914	850514	36.03%	8.224%
6	7.583	758	765	776	rVB	414913	755414	32.00%	7.304%
7	8.059	839	846	855	rVB	72432	124803	5.29%	1.207%
8	8.382	892	901	914	rBV	313361	573614	24.30%	5.546%
9	9.234	1038	1046	1058	rBV	266953	514651	21.80%	4.976%
10	10.879	1319	1326	1334	rVB	90564	171183	7.25%	1.655%
11	13.318	1731	1741	1753	rBV	755637	1215221	51.48%	11.750%
12	14.140	1875	1881	1888	rBV	60166	95240	4.03%	0.921%
13	14.698	1969	1976	1985	rBV2	156860	264607	11.21%	2.559%
14	16.185	2222	2229	2249	rBV2	690386	1038753	44.00%	10.044%
15	17.442	2437	2443	2454	rBV	245281	382093	16.19%	3.695%
16	18.300	2585	2589	2599	rBV3	40344	72575	3.07%	0.702%
17	19.569	2799	2805	2811	rBV3	28941	43848	1.86%	0.424%
18	20.045	2880	2886	2896	rBV	1827526	2360578	100.00%	22.825%
19	21.320	3098	3103	3114	rBV5	16451	40575	1.72%	0.392%
20	21.719	3163	3171	3178	rBV2	292071	485454	20.57%	4.694%
21	25.016	3722	3732	3743	rVB2	161192	468973	19.87%	4.535%

Sum of corrected areas: 10342149

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Misc :
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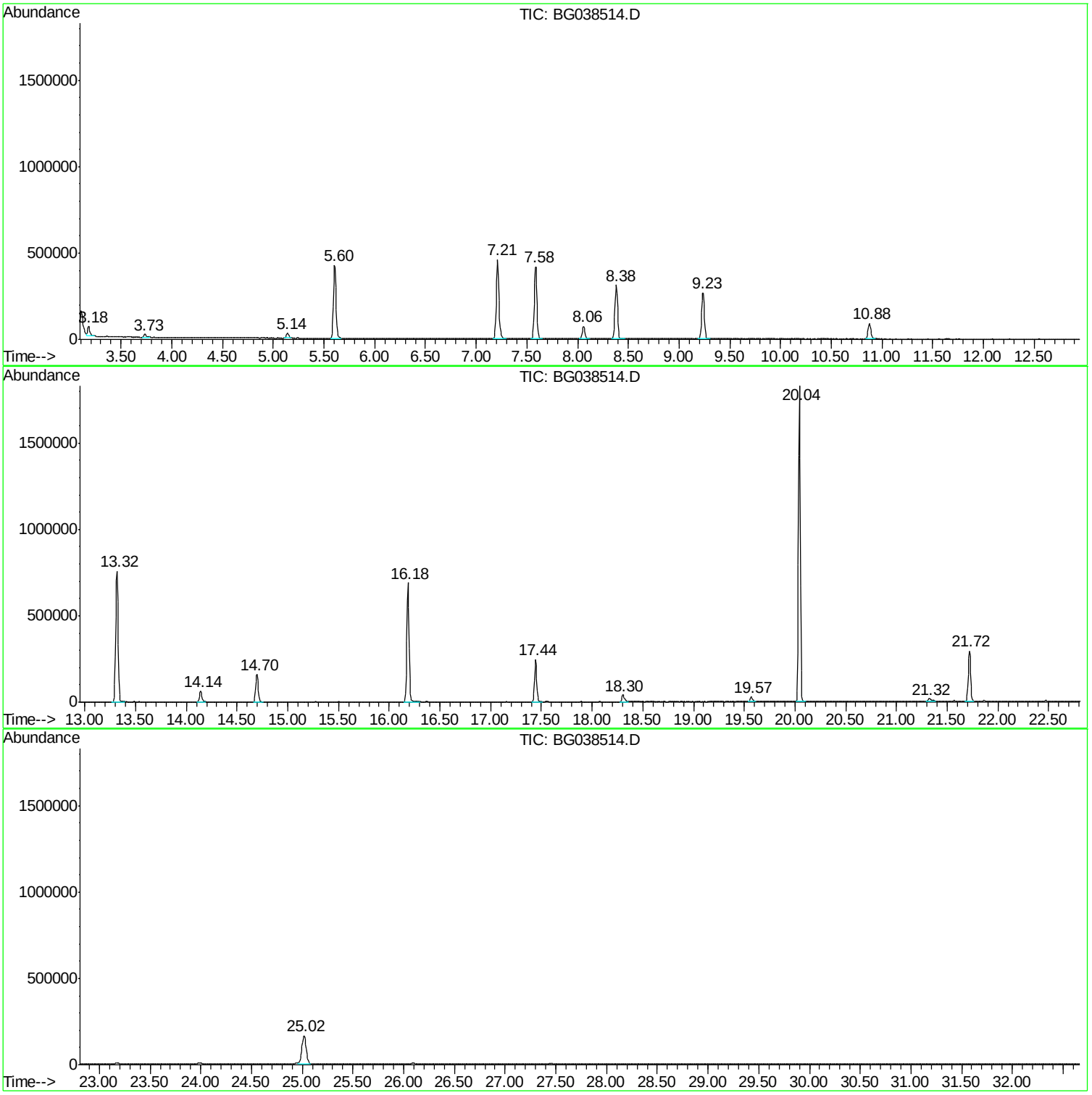
Instrument :
BNA_G
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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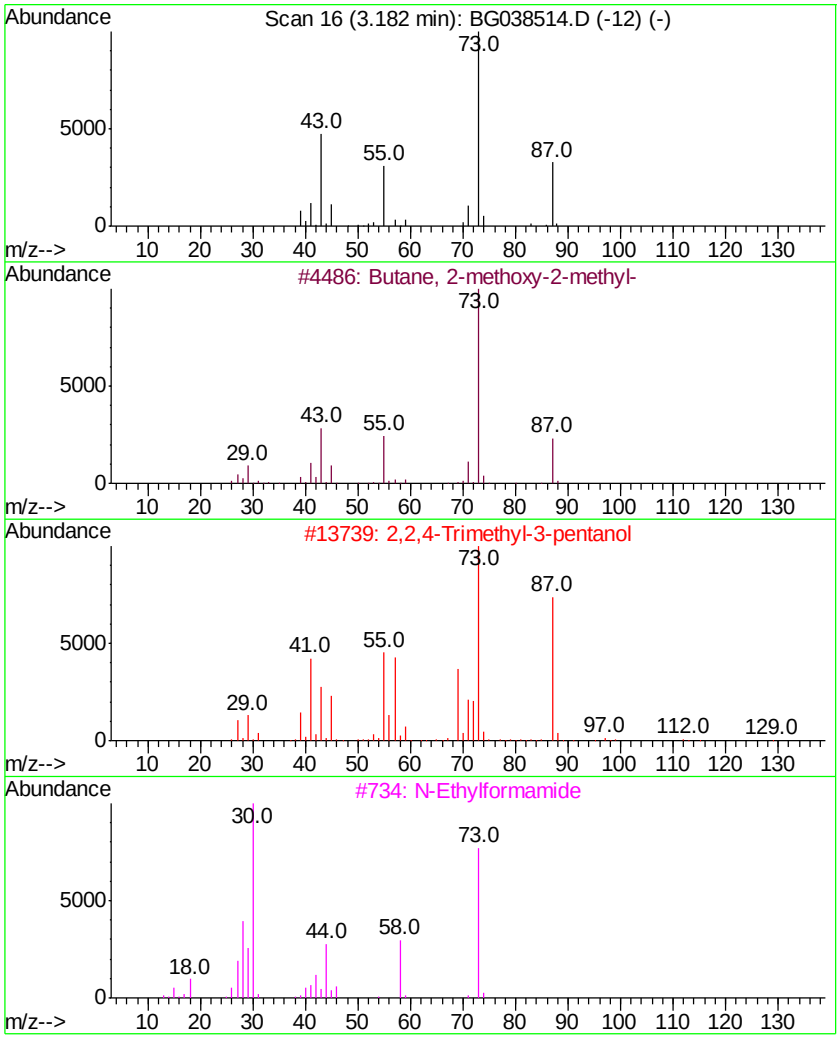
TIC Integration Parameters: LSCINT.P

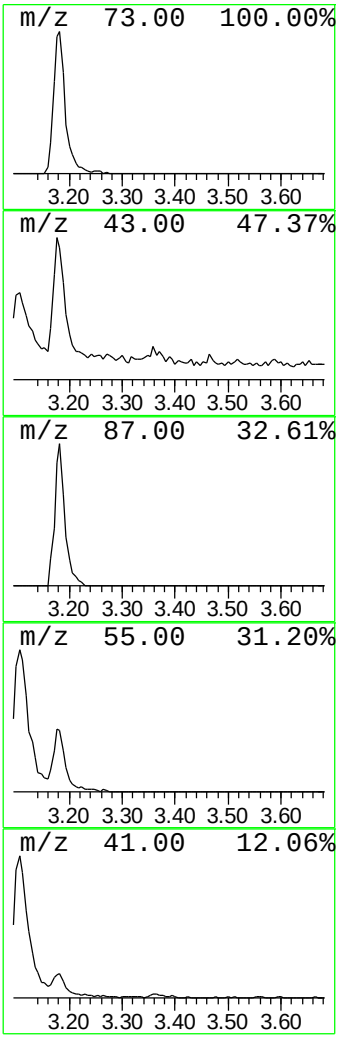
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	14.18 ng	88466	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





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Sample : J6331-13
Misc :
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Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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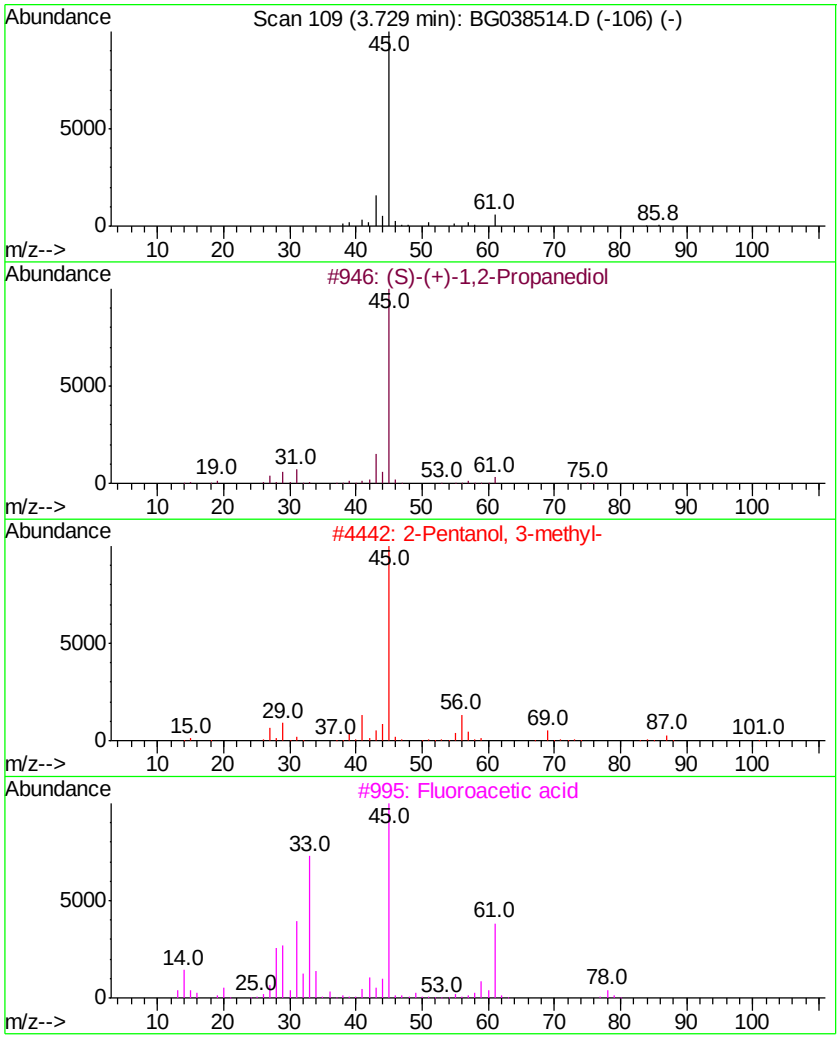
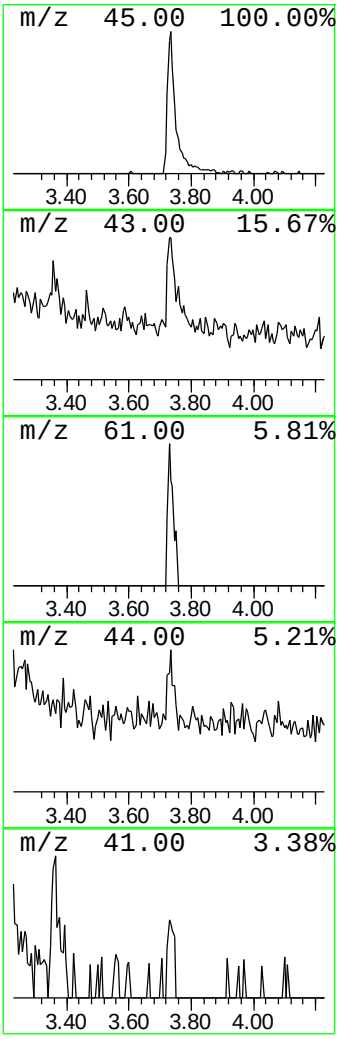
Peak Number 2 unknown3.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	4.51 ng	28153	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9
3	Fluoroacetic acid	78	C2H3FO2	000144-49-0	9
4	2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5	2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	9





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Sample : J6331-13
Misc :
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Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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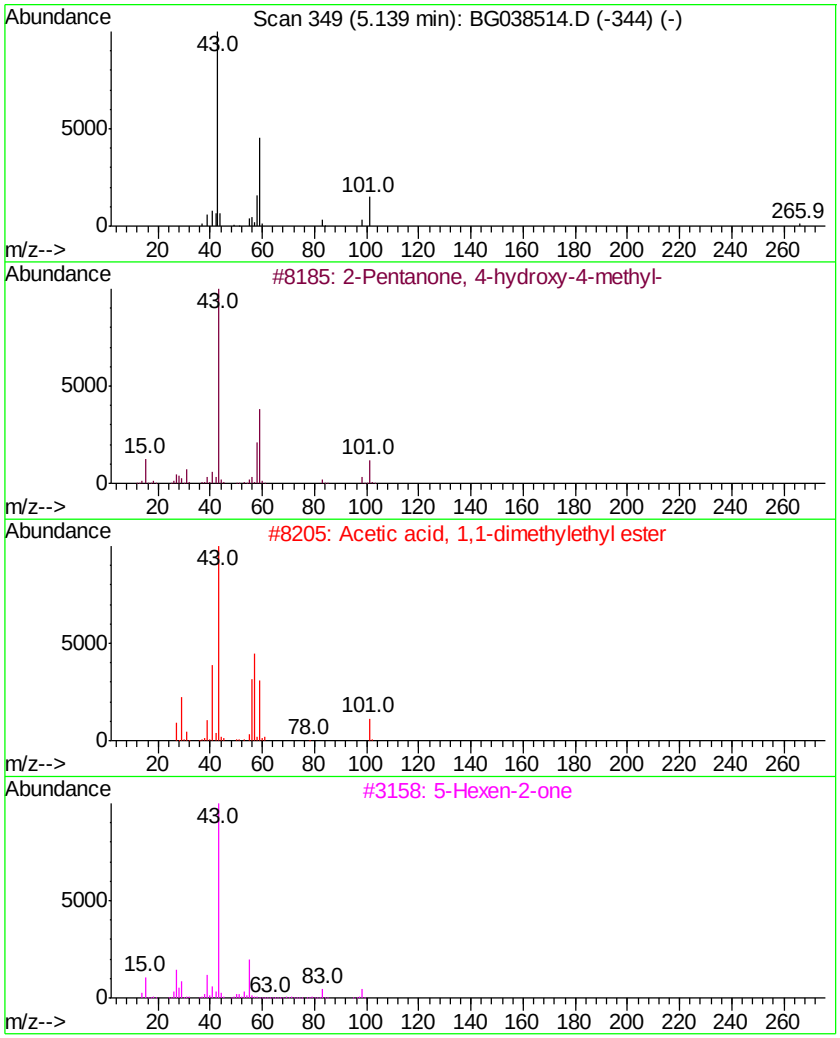
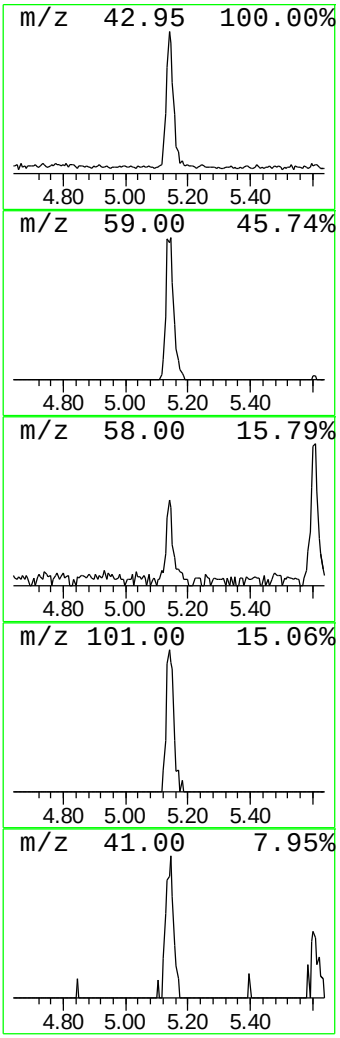
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.17 ng	44726	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Cycloserine	102	C3H6N2O2	000068-41-7	9





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
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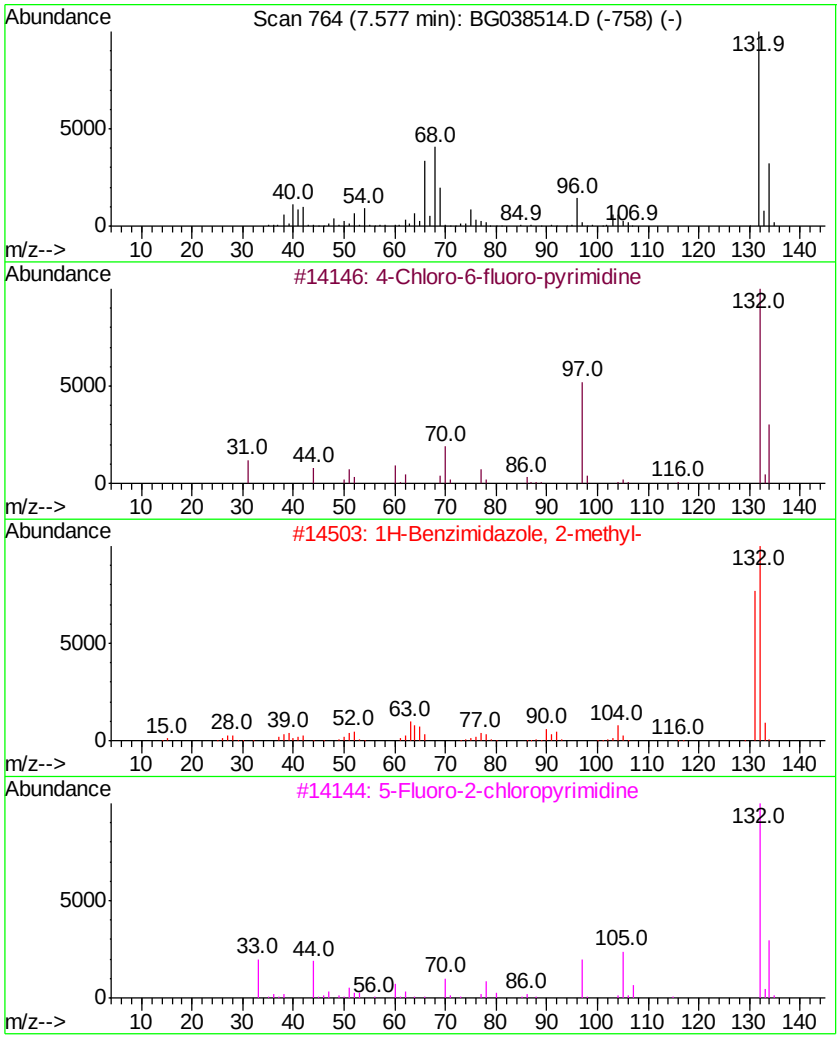
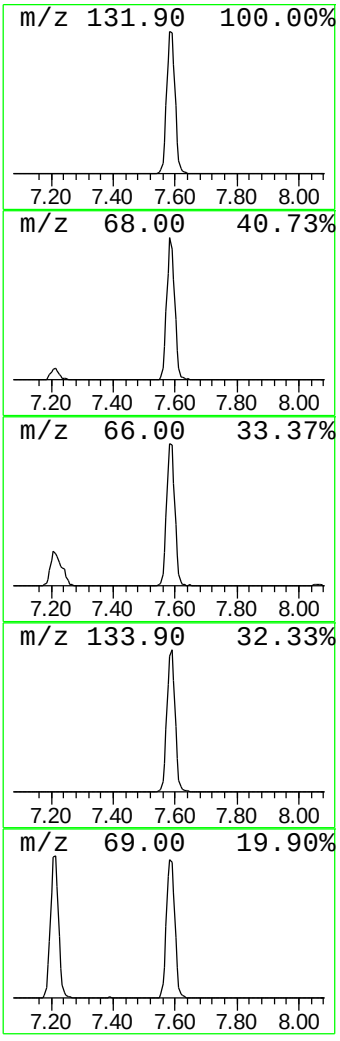
Peak Number 4 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	121.06 ng	755414	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
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Misc :
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Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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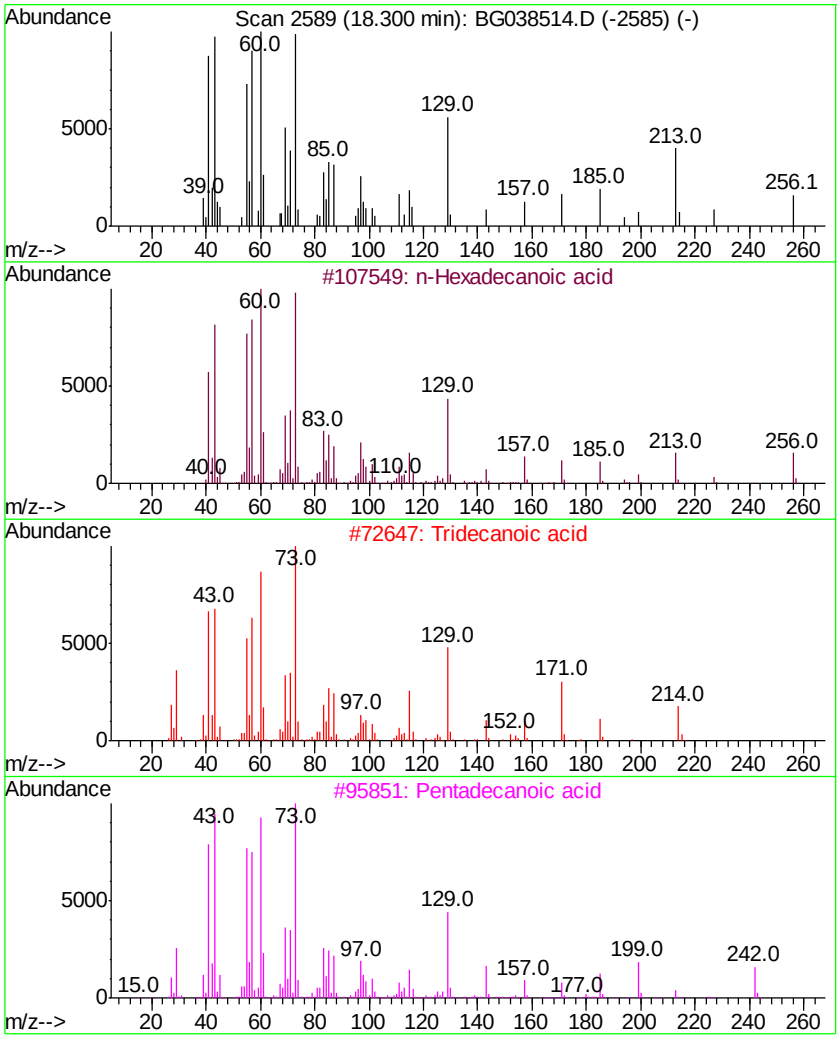
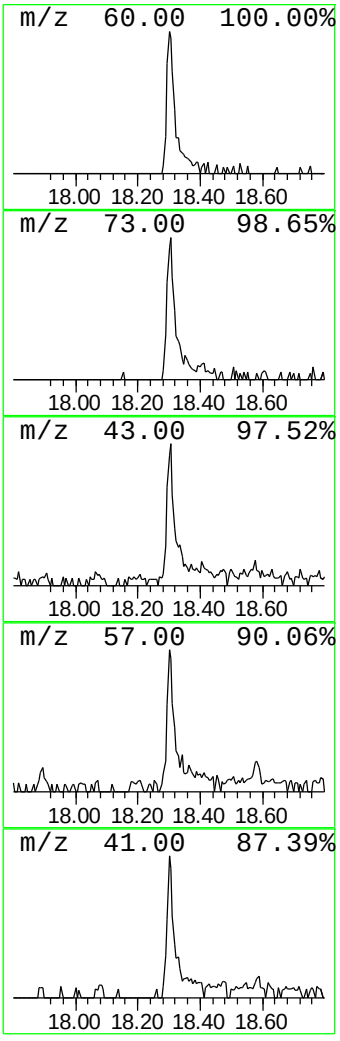
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.80 ng	72575	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

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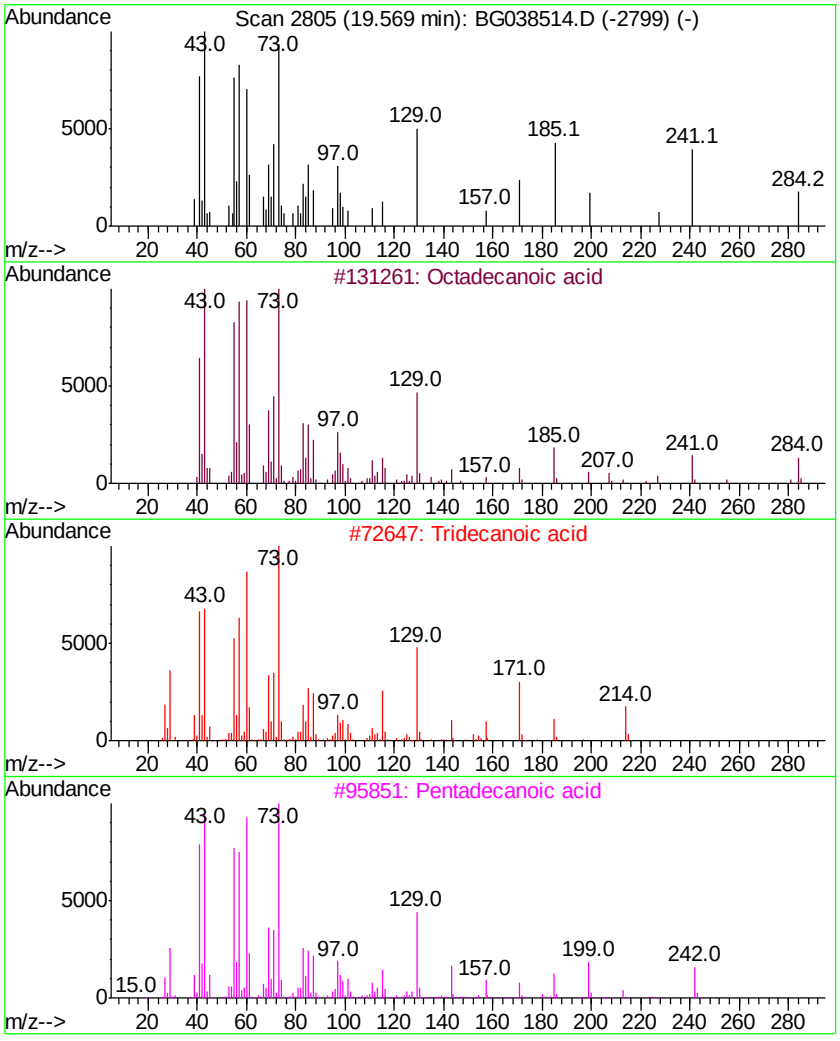
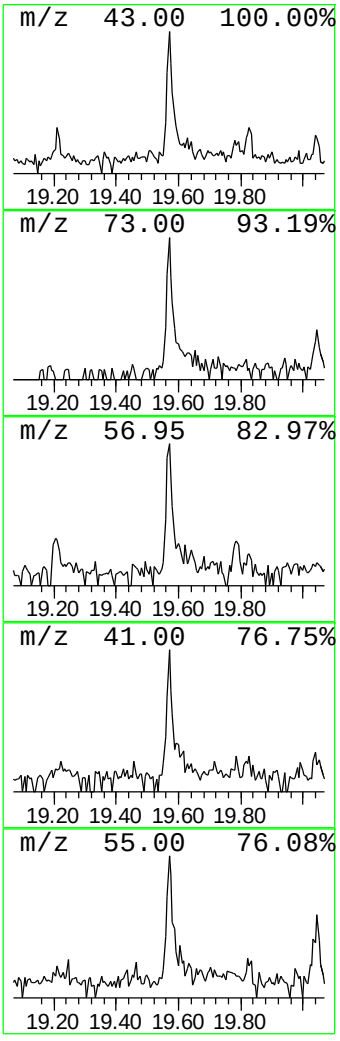
****

Peak Number 7 unknown19.57 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	2.30 ng	43848	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	49
2	Tridecanoic acid	214	C13H26O2	000638-53-9	47
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35
5	Undecanoic acid	186	C11H22O2	000112-37-8	35





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
Butane, 2-methoxy...	3.18	14.2	ng	88466	1	8.06	124803	20.0
unknown3.73	3.73	4.5	ng	28153	1	8.06	124803	20.0
2-Pentanone, 4-hy...	5.14	7.2	ng	44726	1	8.06	124803	20.0
unknown7.58	7.58	121.1	ng	755414	1	8.06	124803	20.0
n-Hexadecanoic acid	18.30	3.8	ng	72575	4	17.44	382093	20.0
unknown19.57	19.57	2.3	ng	43848	4	17.44	382093	20.0