LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038519.D
Acq On : 13 Dec 2018 4:36
Operator : JU/SJ
Sample : J6331-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2

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	3.179	11	15	28	rVB	65115	111641	6.02%	1.229%
2	3.731	106	109	119	rVB	12636	23435	1.26%	0.258%
3	5.141	344	349	355	rBV	24426	38351	2.07%	0.422%
4	5.605	421	428	439	rBV	385462	630834	34.02%	6.943%
5	7.209	693	701	715	rBV	403862	752009	40.56%	8.277%
6	7.585	758	765	775	rBV	373439	667103	35.98%	7.342%
7	8.061	839	846	856	rVB	65910	119446	6.44%	1.315%
8	8.378	893	900	910	rVB	270669	497781	26.85%	5.479%
9	9.236	1036	1046	1058	rBV	241115	455634	24.57%	5.015%
10	10.875	1319	1325	1334	rBV	87343	163643	8.83%	1.801%
11	13.314	1734	1740	1755	rBV	650942	1033765	55.76%	11.378%
12	14.142	1875	1881	1891	rBV	61174	99400	5.36%	1.094%
13	14.695	1969	1975	1985	rVB2	152322	246923	13.32%	2.718%
14	16.187	2222	2229	2249	rBV3	560604	899076	48.49%	9.895%
15	17.444	2436	2443	2454	rBV2	222545	346400	18.68%	3.813%
16	18.302	2584	2589	2599	rBV	74877	130182	7.02%	1.433%
17	19.571	2800	2805	2814	rBV	55814	92160	4.97%	1.014%
18	20.047	2879	2886	2893	rBV	1323635	1854072	100.00%	20.406%
19	21.316	3097	3102	3116	rBV2	47644	102391	5.52%	1.127%
20	21.722	3163	3171	3179	rBV	247134	418367	22.56%	4.605%
21	25.018	3722	3732	3744	rVB2	141822	403233	21.75%	4.438%

Sum of corrected areas: 9085846

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Misc :
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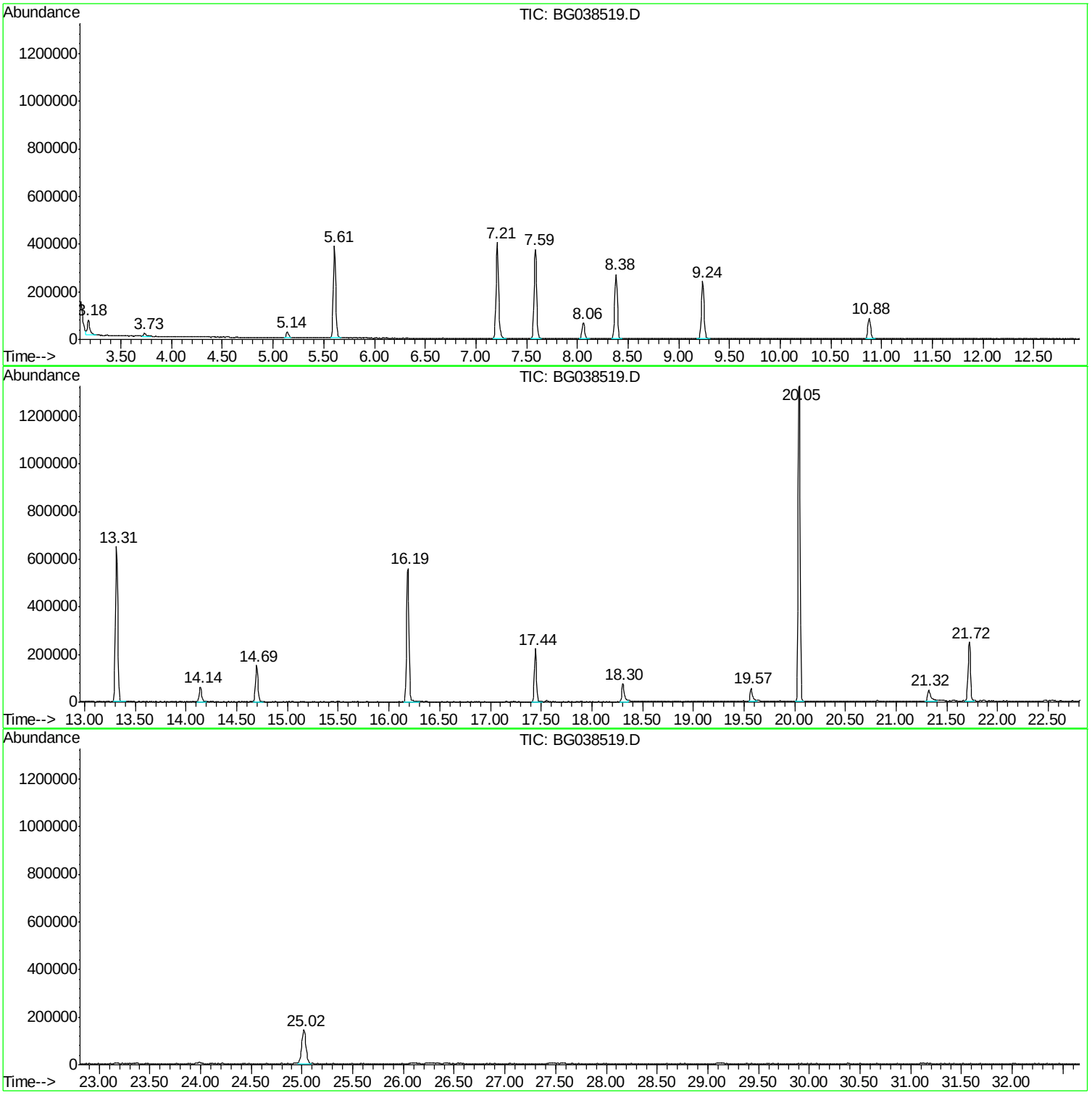
Instrument :
BNA_G
ClientSampleId :
TP-2

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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Data File : BG038519.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

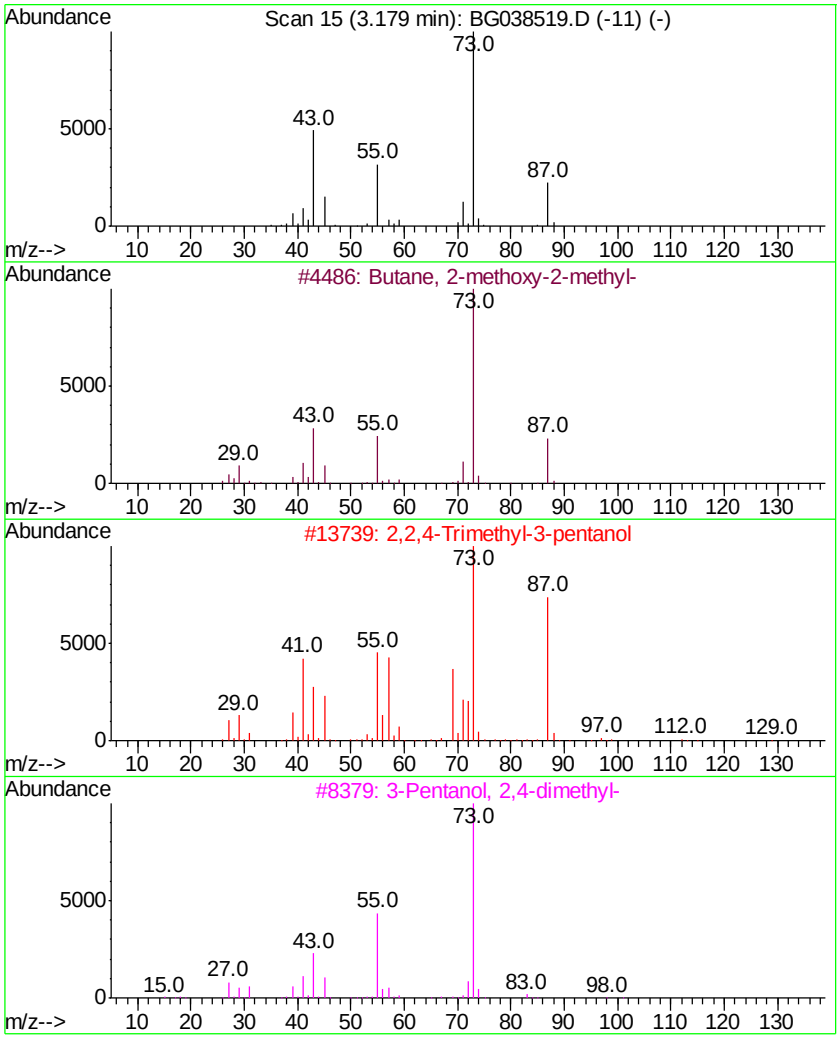
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

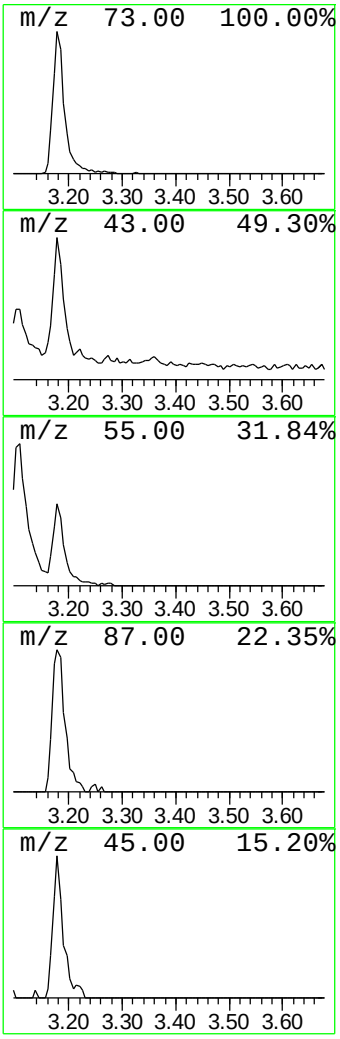
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	18.69 ng	111641	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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2

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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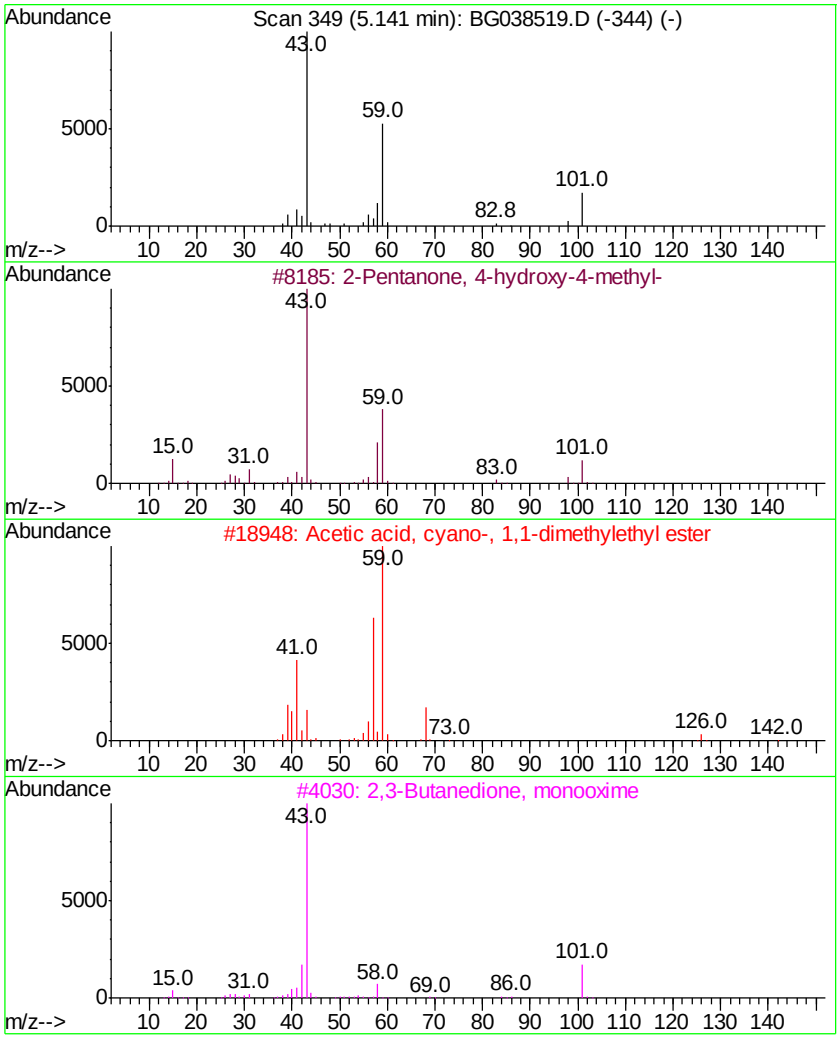
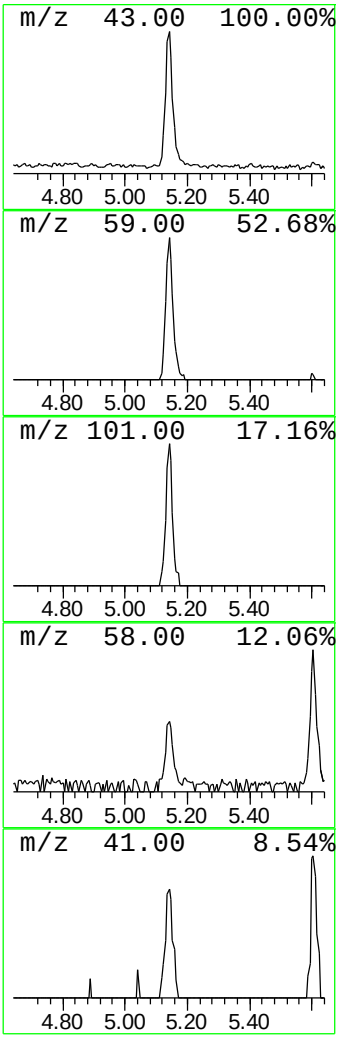
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.42 ng	38351	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	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038519.D
Acq On : 13 Dec 2018 4:36
Operator : JU/SJ
Sample : J6331-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2

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

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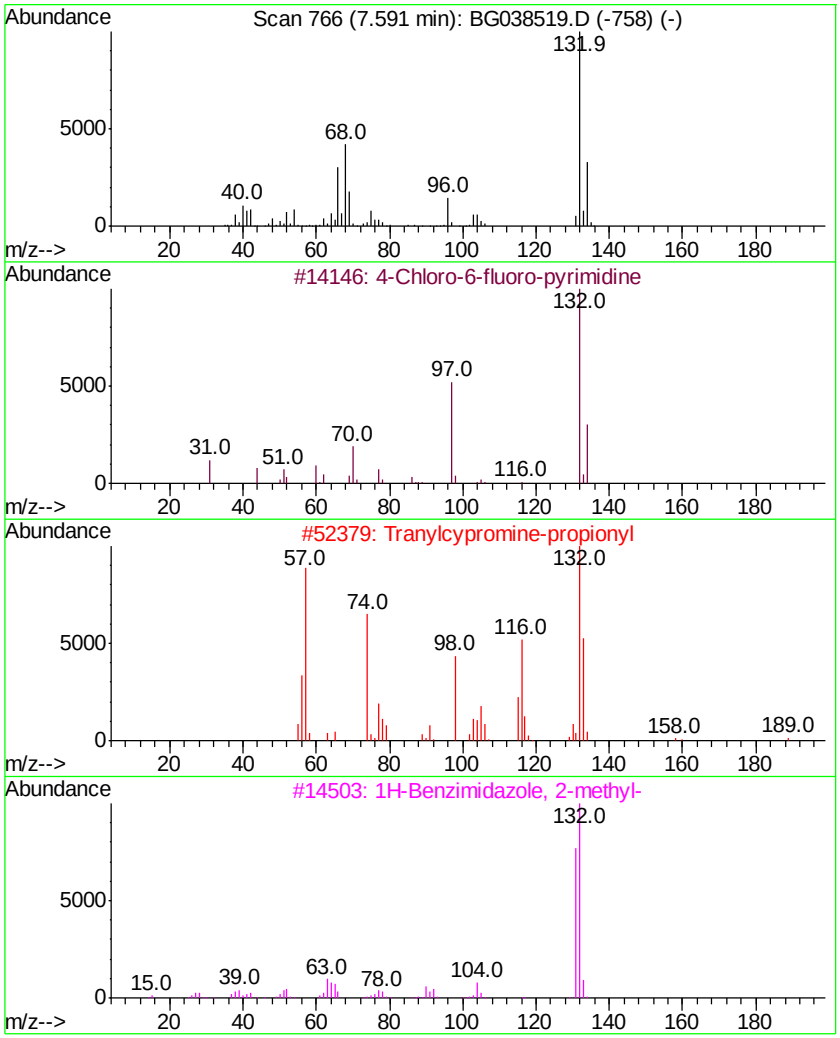
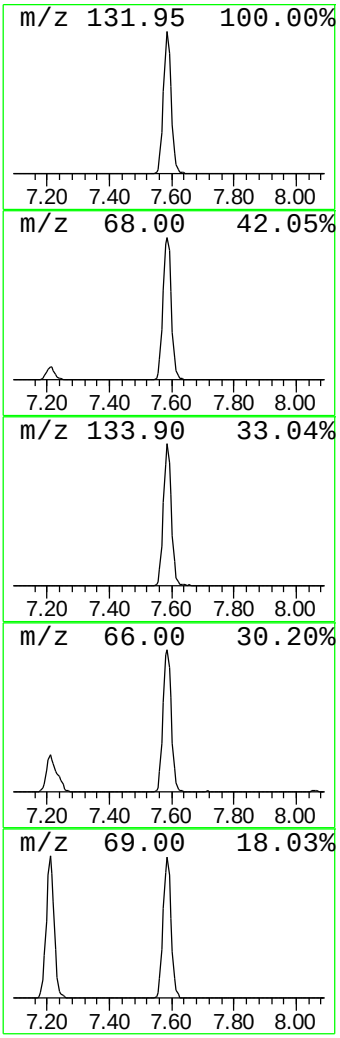
****

Peak Number 4 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	111.70 ng	667103	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
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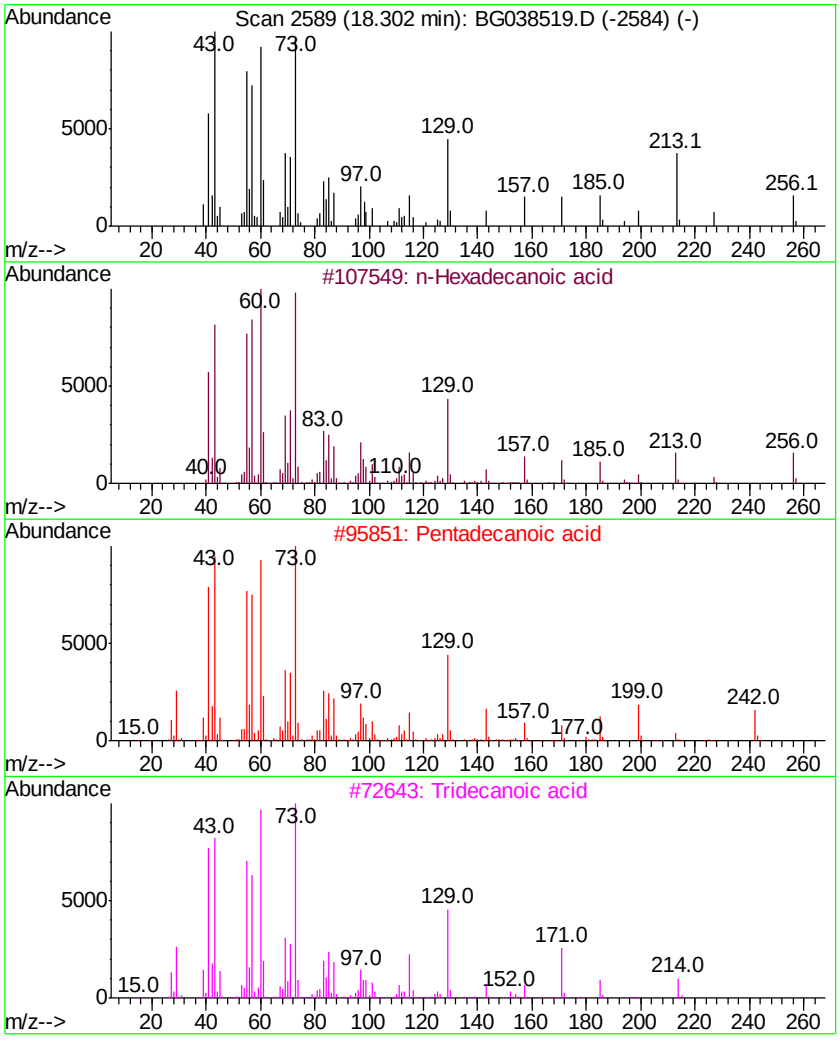
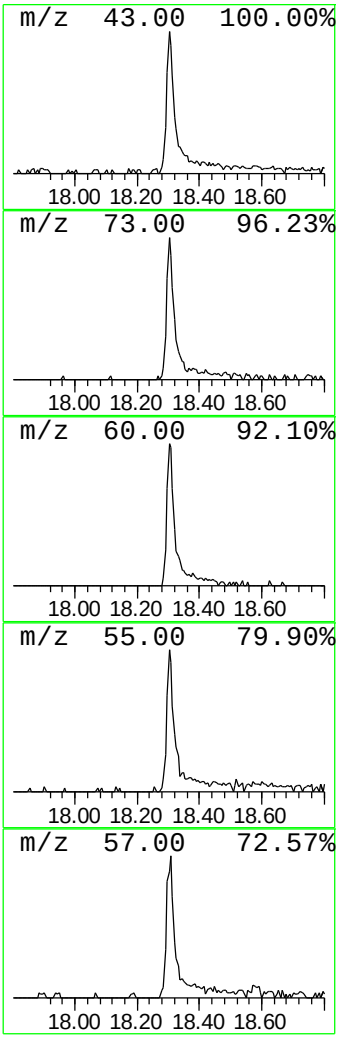
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	7.52 ng	130182	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Library Search Compound Report

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Operator : JU/SJ
Sample : J6331-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2

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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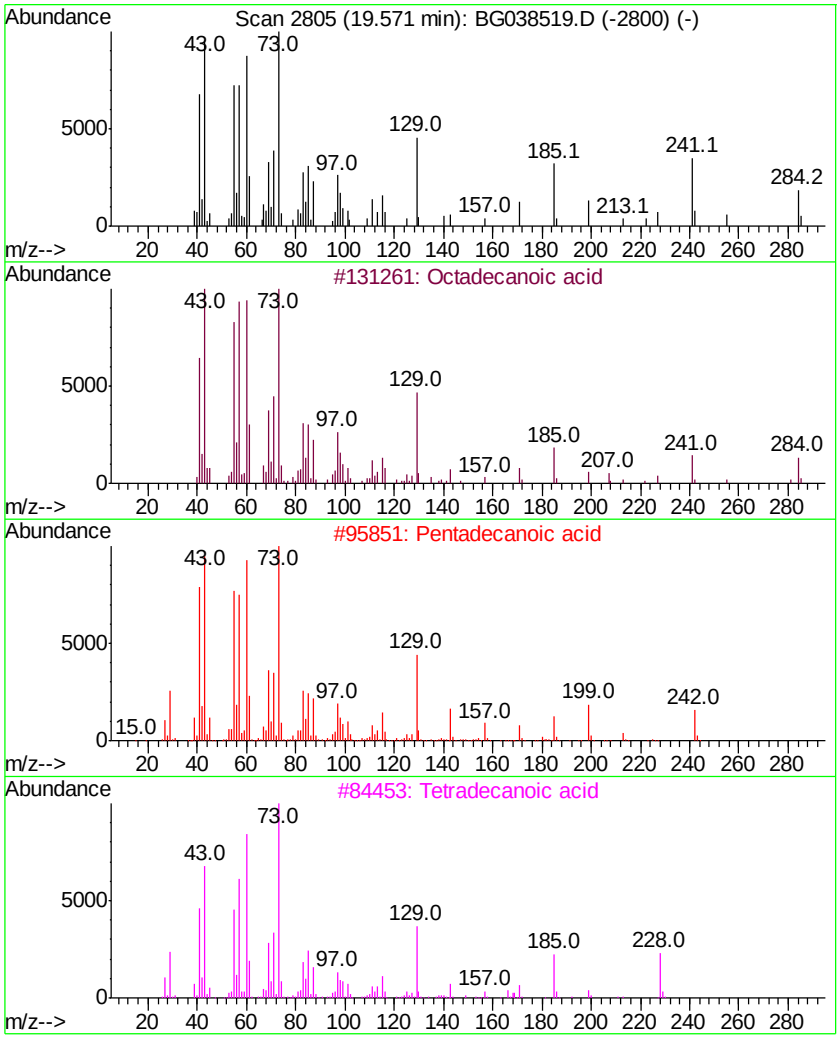
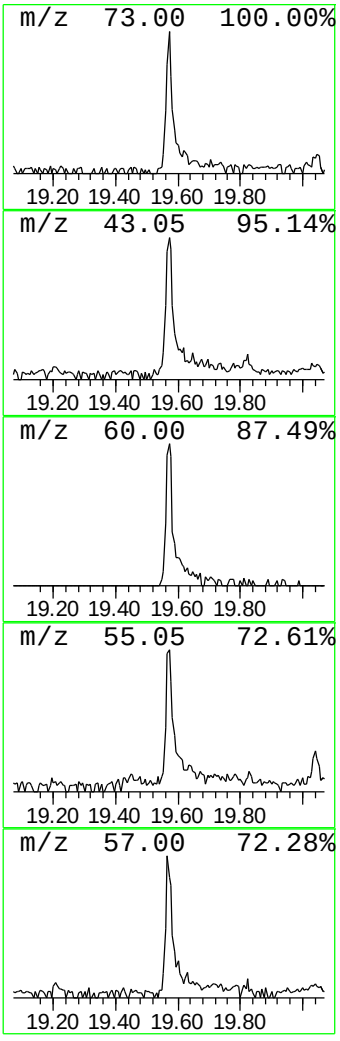
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	5.32 ng	92160	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





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ClientSampleId : TP-2

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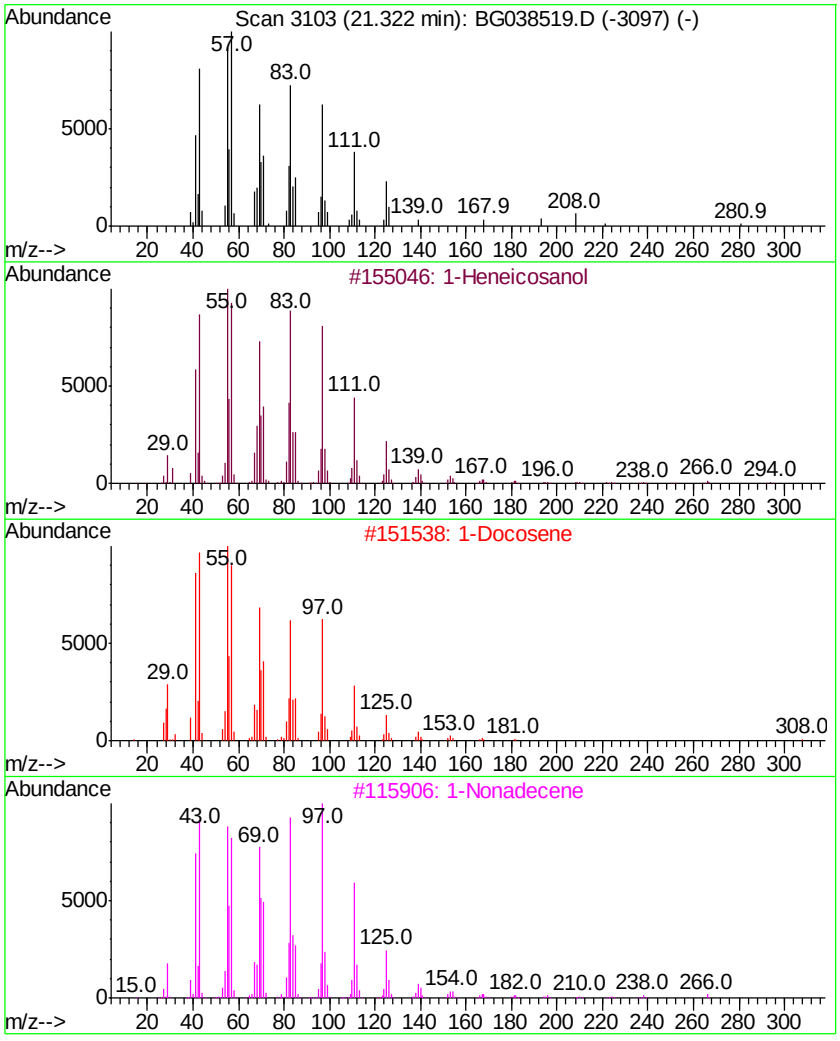
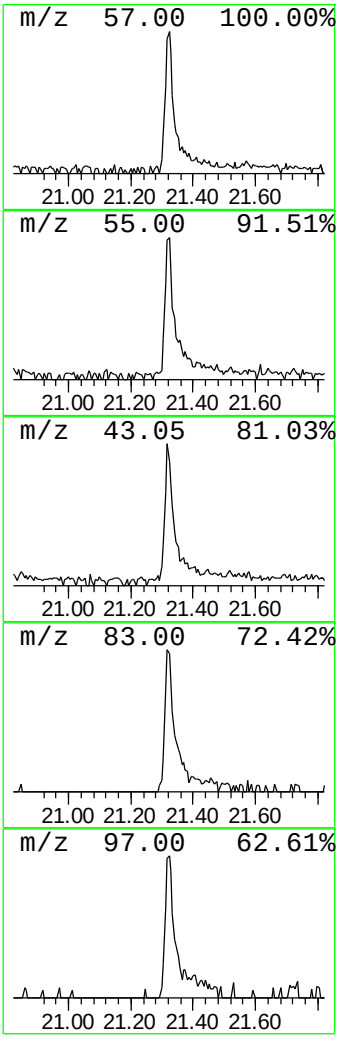
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	4.89 ng	102391	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Docosene	308	C22H44	001599-67-3	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90





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
Butane, 2-methoxy...	3.18	18.7	ng	111641	1	8.06	119446	20.0
2-Pentanone, 4-hy...	5.14	6.4	ng	38351	1	8.06	119446	20.0
unknown7.59	7.59	111.7	ng	667103	1	8.06	119446	20.0
n-Hexadecanoic acid	18.30	7.5	ng	130182	4	17.44	346400	20.0
Octadecanoic acid	19.57	5.3	ng	92160	4	17.44	346400	20.0
1-Heneicosanol	21.32	4.9	ng	102391	5	21.72	418367	20.0