LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021121\
Data File : BG048141.D
Acq On : 11 Feb 2021 18:33
Operator : CG/JU
Sample : M1388-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

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-BG021021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.659	388	395	402	rBV	437459	695484	14.11%	3.509%
2	7.251	659	666	677	rVB	264670	496416	10.07%	2.504%
3	8.103	804	811	817	rBV	163868	275703	5.60%	1.391%
4	9.266	1001	1009	1018	rBV	625547	1106760	22.46%	5.584%
5	9.419	1025	1035	1044	rBV3	54107	99055	2.01%	0.500%
6	10.676	1243	1249	1260	rBV2	26182	54328	1.10%	0.274%
7	10.917	1282	1290	1297	rBV	211753	377650	7.66%	1.905%
8	11.704	1417	1424	1435	rBV2	82462	174510	3.54%	0.880%
9	13.350	1697	1704	1713	rVB	1714965	2638110	53.54%	13.309%
10	14.166	1839	1843	1853	rVB	57914	100182	2.03%	0.505%
11	14.724	1929	1938	1944	rBV	409718	626643	12.72%	3.161%
12	15.130	2002	2007	2017	rBV3	45404	93031	1.89%	0.469%
13	16.211	2184	2191	2200	rBV	1668343	2587895	52.52%	13.056%
14	17.468	2398	2405	2411	rBV	555724	843203	17.11%	4.254%
15	18.261	2536	2540	2544	rVB2	35593	50286	1.02%	0.254%
16	18.355	2550	2556	2571	rBV	612389	1061640	21.55%	5.356%
17	19.613	2766	2770	2784	rBV	393455	675540	13.71%	3.408%
18	20.071	2841	2848	2857	rBV	3852436	4927295	100.00%	24.858%
19	21.370	3064	3069	3079	rBV	328650	596671	12.11%	3.010%
20	21.734	3125	3131	3139	rVB	622859	998064	20.26%	5.035%
21	22.921	3329	3333	3340	rVB3	63475	123299	2.50%	0.622%
22	23.250	3384	3389	3396	rVB4	37814	66725	1.35%	0.337%
23	24.066	3523	3528	3535	rVB4	38968	78389	1.59%	0.395%
24	25.001	3677	3687	3701	rVB2	348948	1074747	21.81%	5.422%

Sum of corrected areas: 19821626

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Misc :
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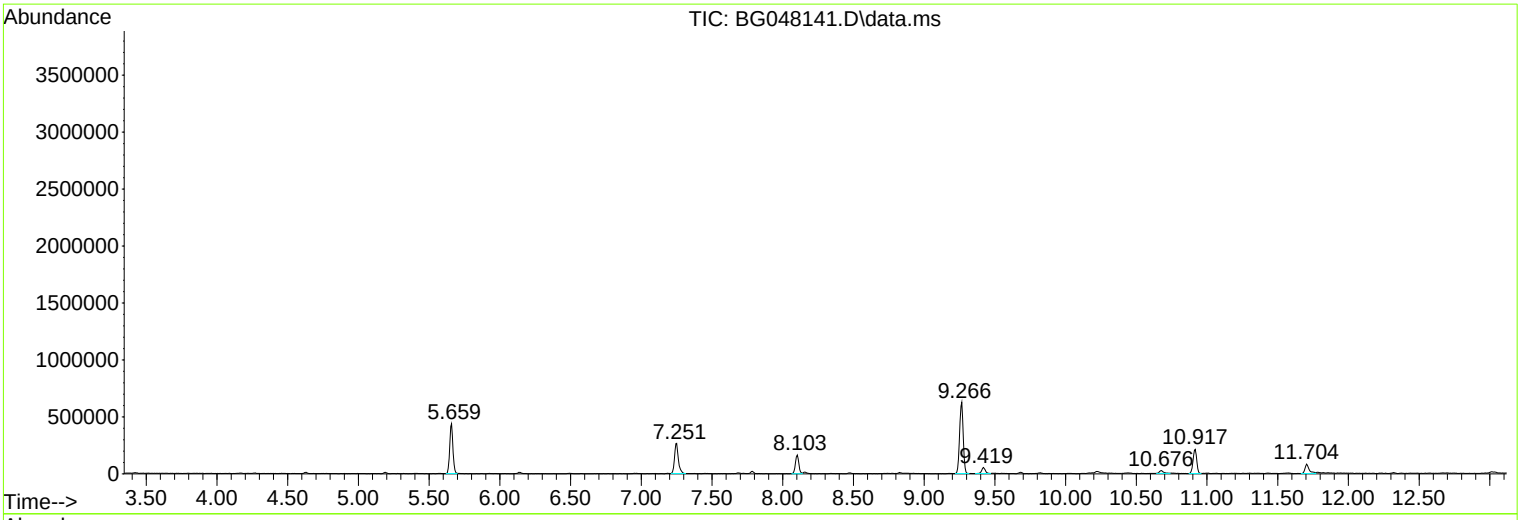
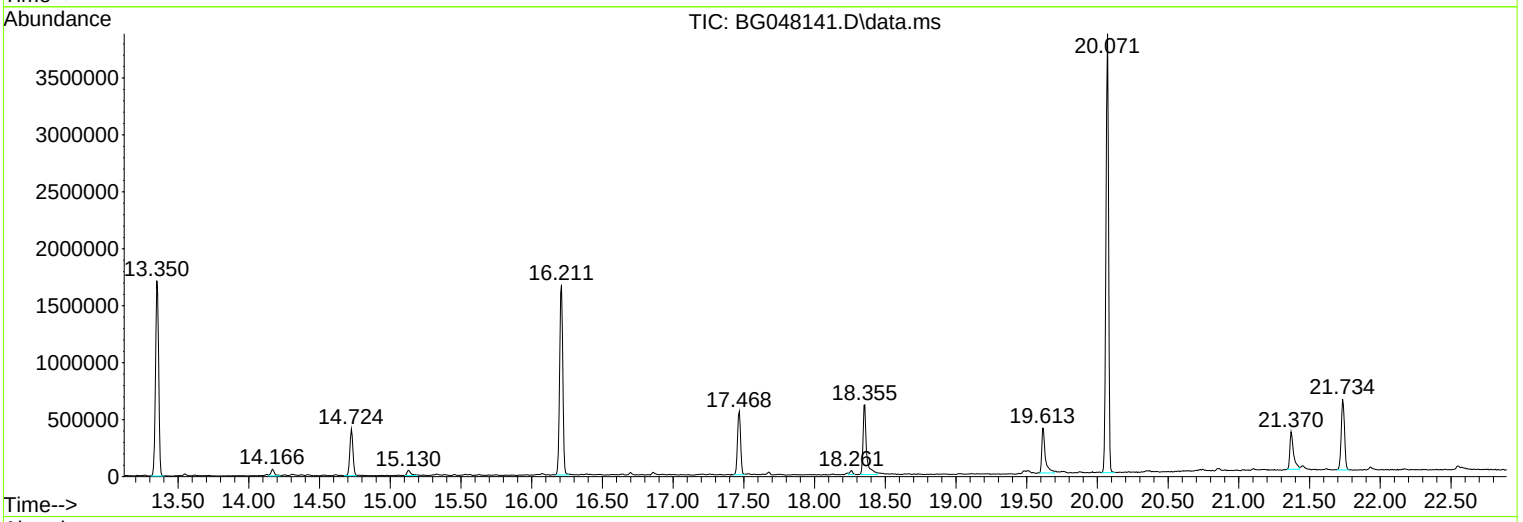
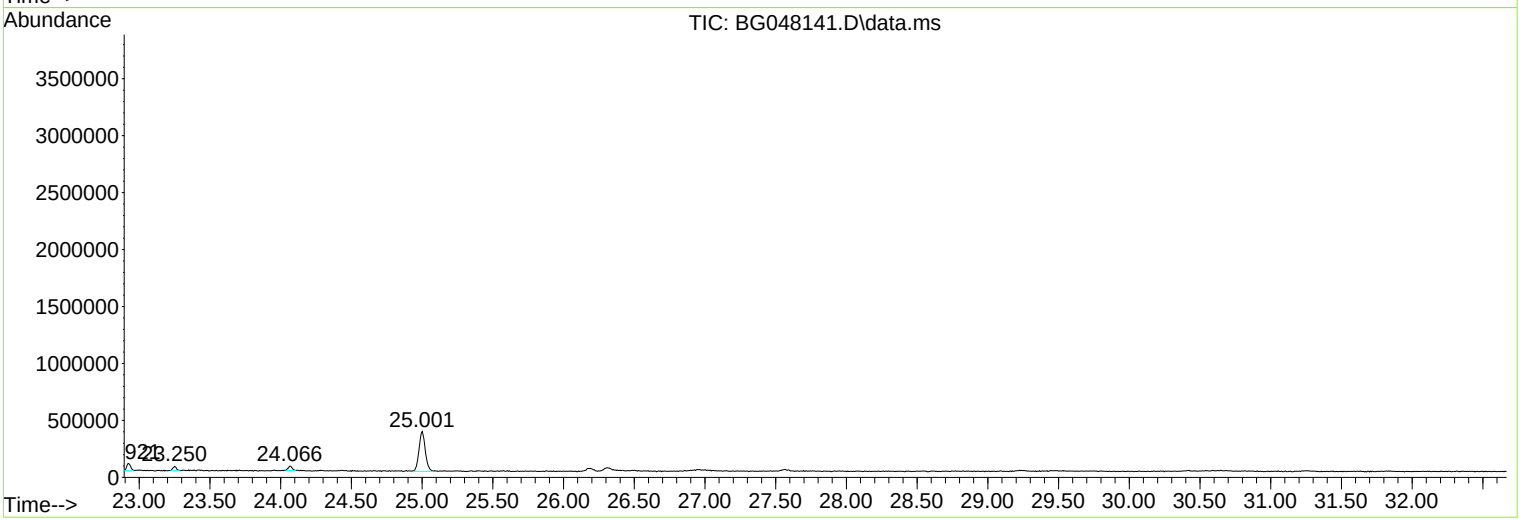
Instrument :
BNA_G
ClientSampleId :
NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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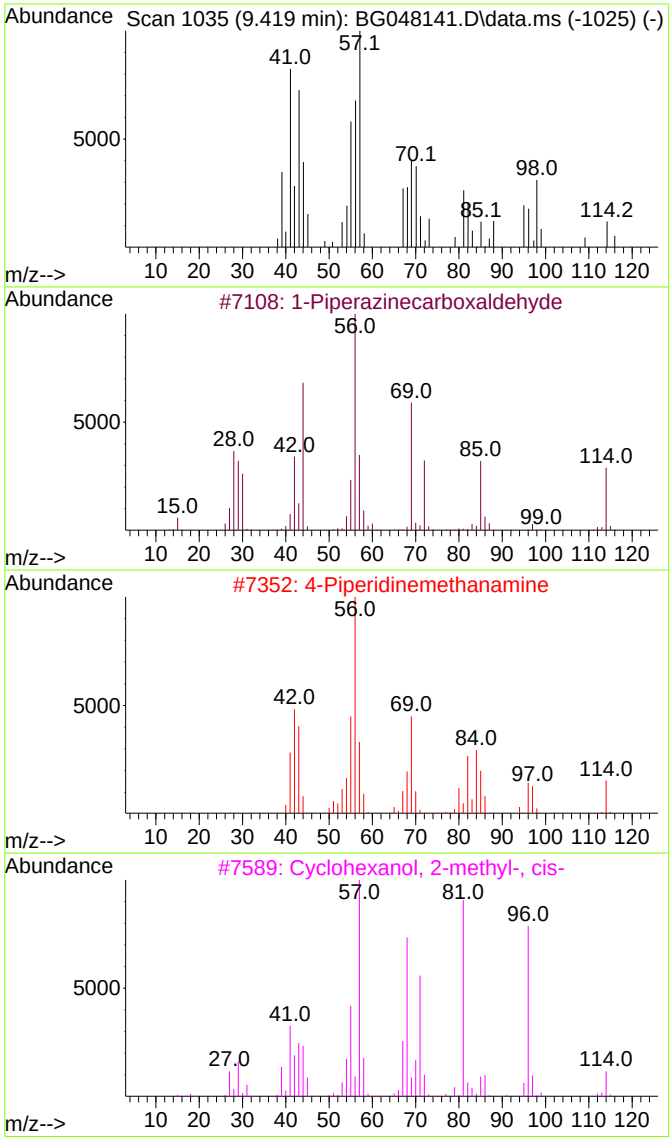
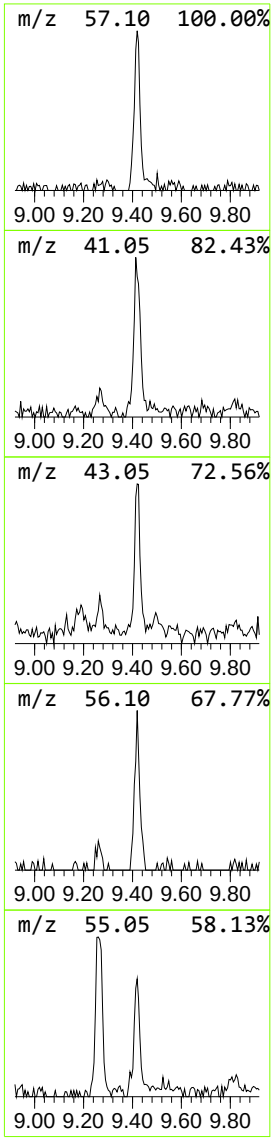
Peak Number 1 unknown9.419 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.419	7.19 ng	99055	1,4-Dichlorobenzene-d4	8.103

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Piperazinecarboxaldehyde	114	C5H10N2O	007755-92-2	35
2	4-Piperidinemethanamine	114	C6H14N2	007144-05-0	30
3	Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	25
4	6-Hepten-1-ol, 3-methyl-	128	C8H16O	004048-32-2	22
5	Cyclooctyl alcohol	128	C8H16O	000696-71-9	22





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Data File : BG048141.D
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Operator : CG/JU
Sample : M1388-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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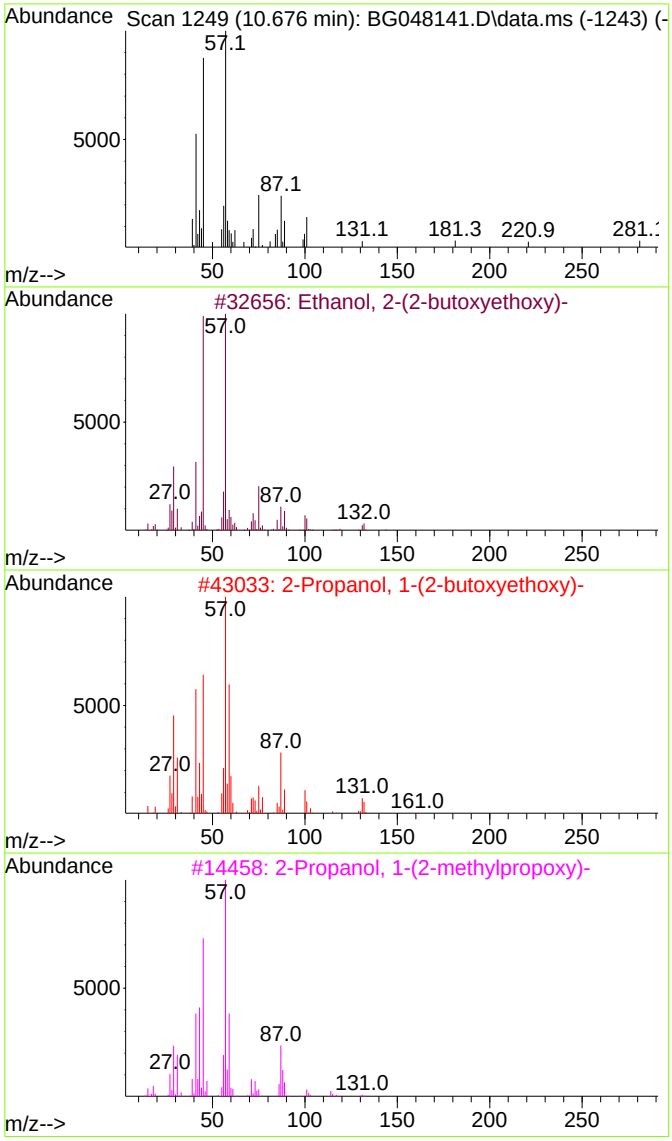
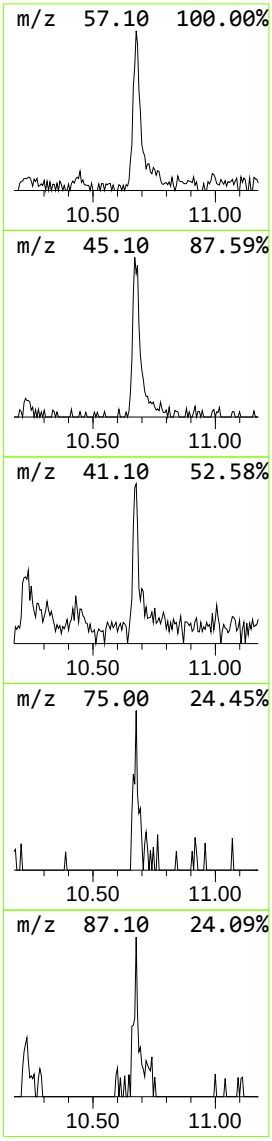
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.676	2.88 ng	54328	Naphthalene-d8	10.917

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	59
2	2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	56
3	2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	45
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	42





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Acq On : 11 Feb 2021 18:33
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Sample : M1388-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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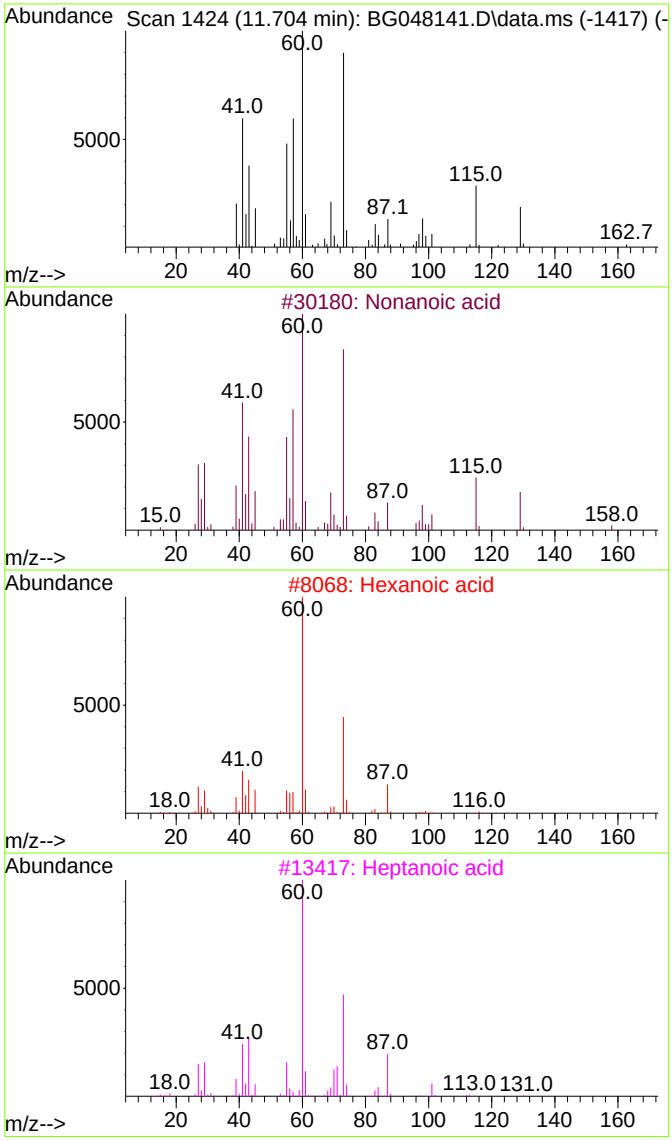
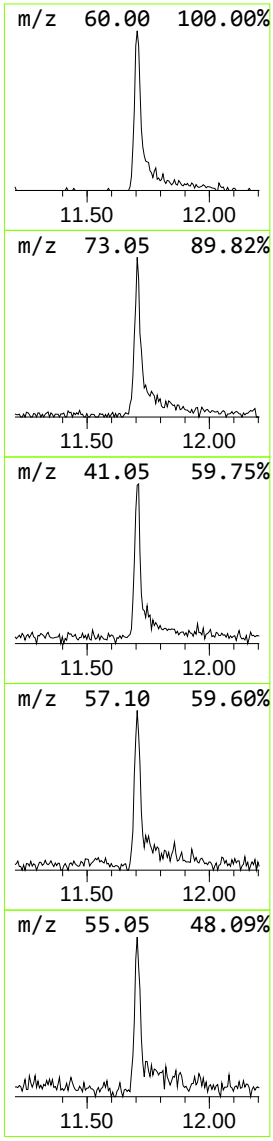
Peak Number 3 Nonanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	9.24 ng	174510	Naphthalene-d8	10.917

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	91
2	Hexanoic acid	116	C6H12O2	000142-62-1	52
3	Heptanoic acid	130	C7H14O2	000111-14-8	47
4	Octanoic acid	144	C8H16O2	000124-07-2	45
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG021121\
Data File : BG048141.D
Acq On : 11 Feb 2021 18:33
Operator : CG/JU
Sample : M1388-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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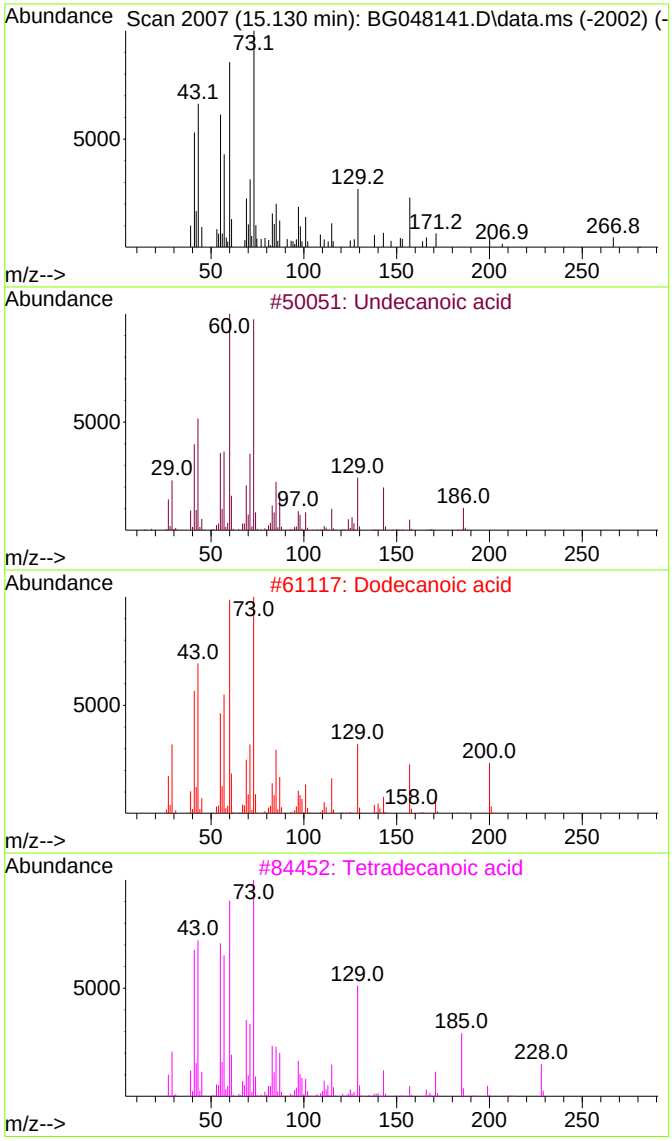
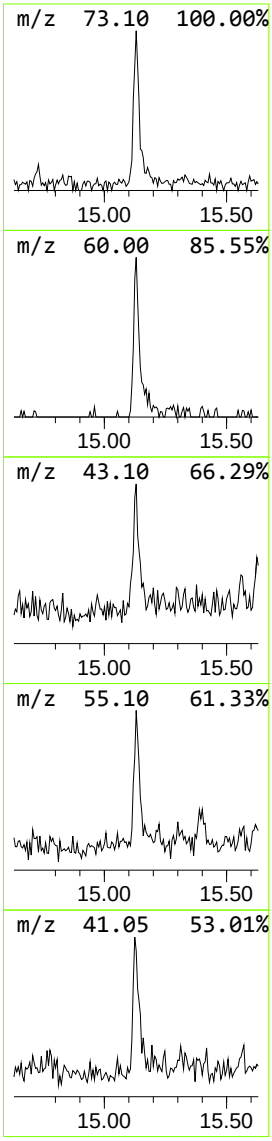
Peak Number 4 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.130	2.97 ng	93031	Acenaphthene-d10	14.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86
2	Dodecanoic acid	200	C12H24O2	000143-07-7	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BG048141.D
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Operator : CG/JU
Sample : M1388-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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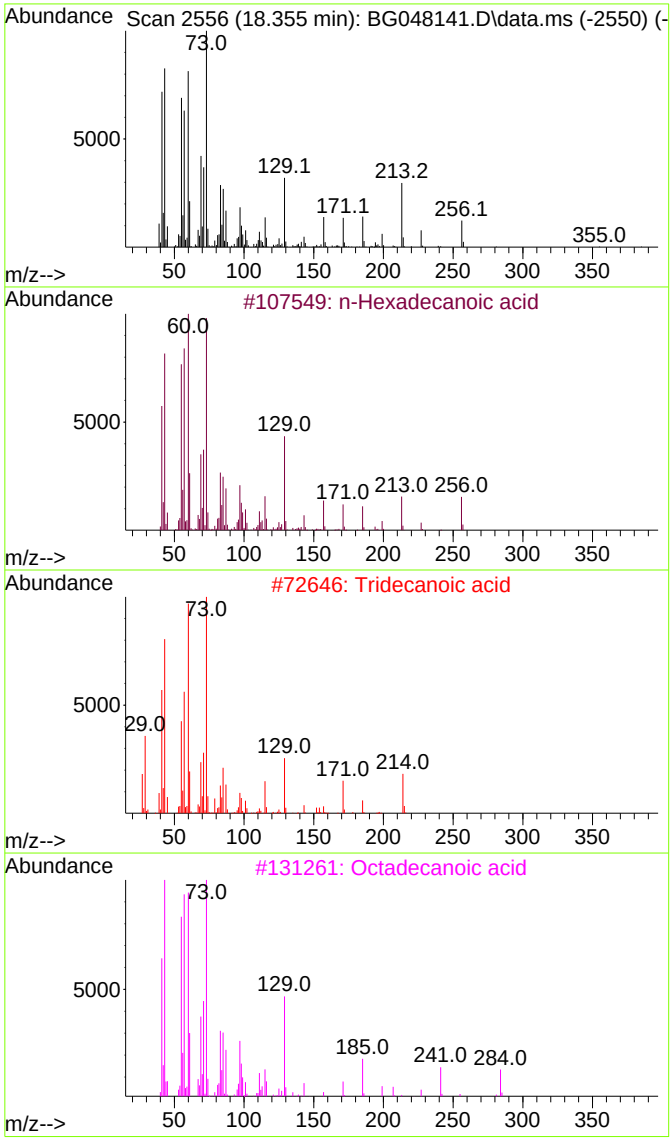
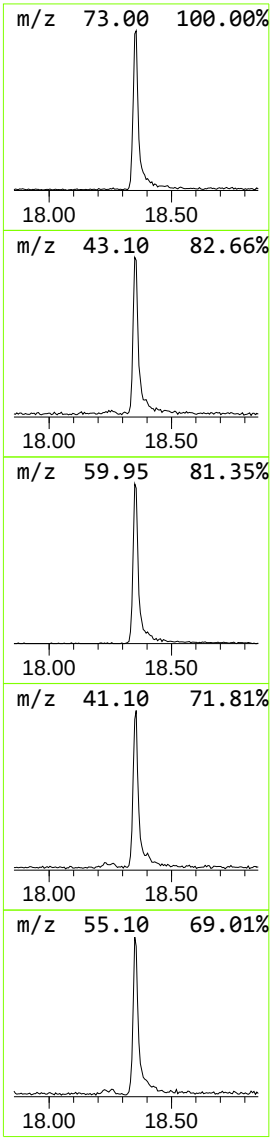
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.355	25.18 ng	1061640	Phenanthrene-d10	17.468

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	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
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TIC Library : C:\Database\NIST11.L
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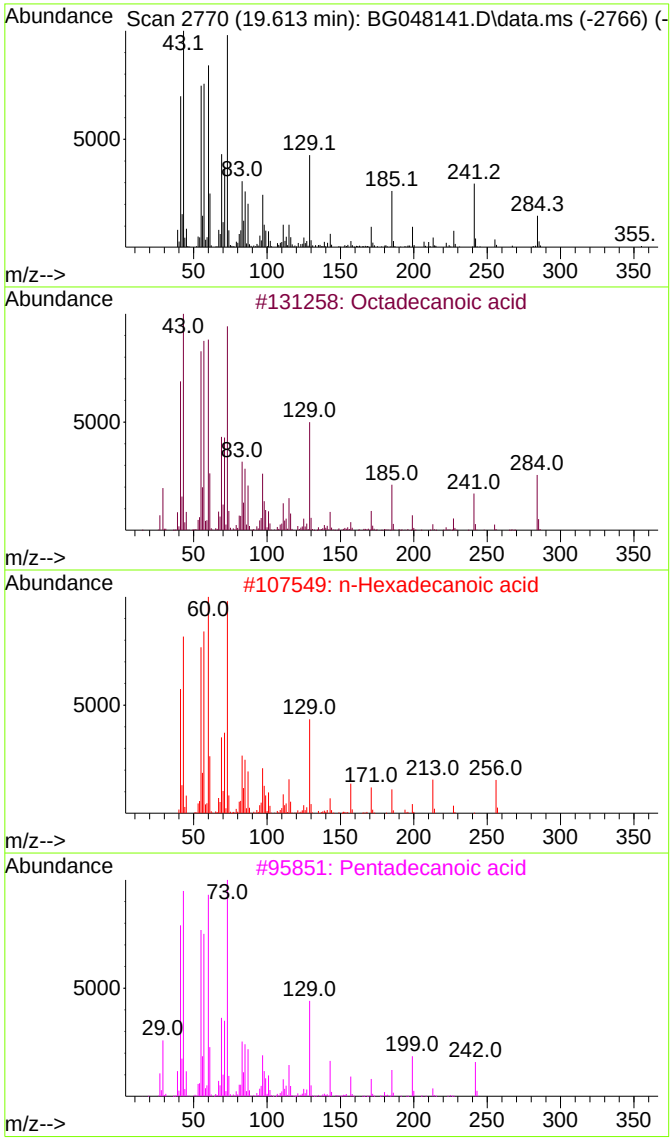
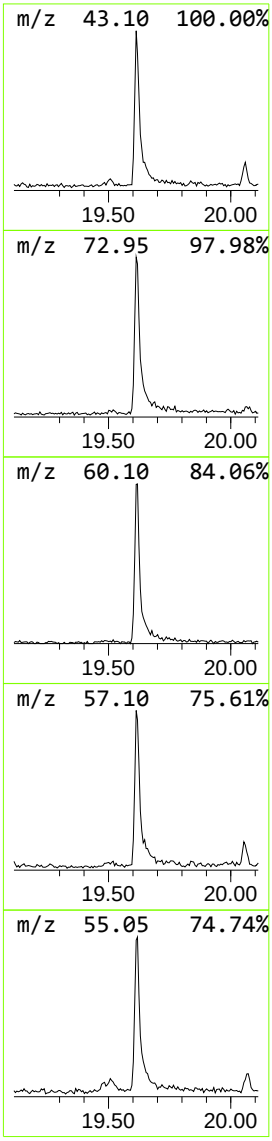
Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.613	13.54 ng	675540	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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ClientSampleId :
NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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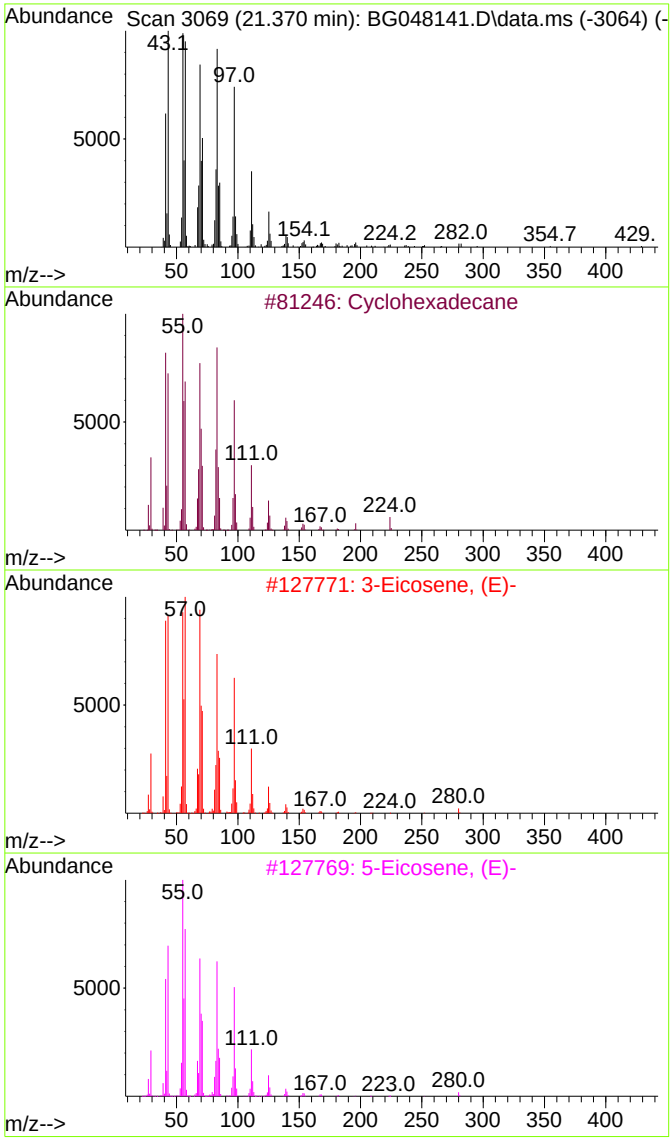
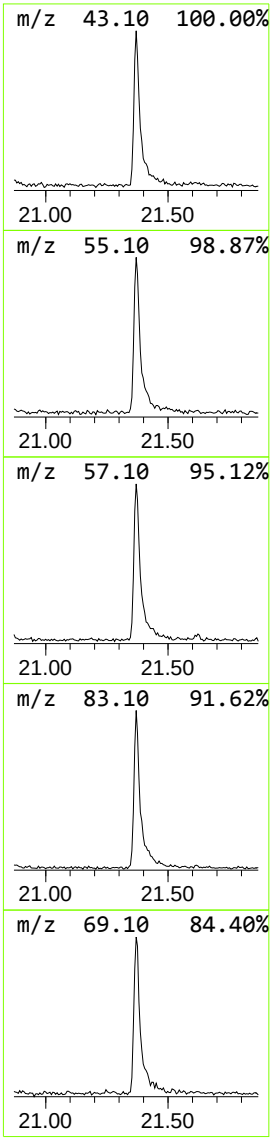
Peak Number 7 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.370	11.96 ng	596671	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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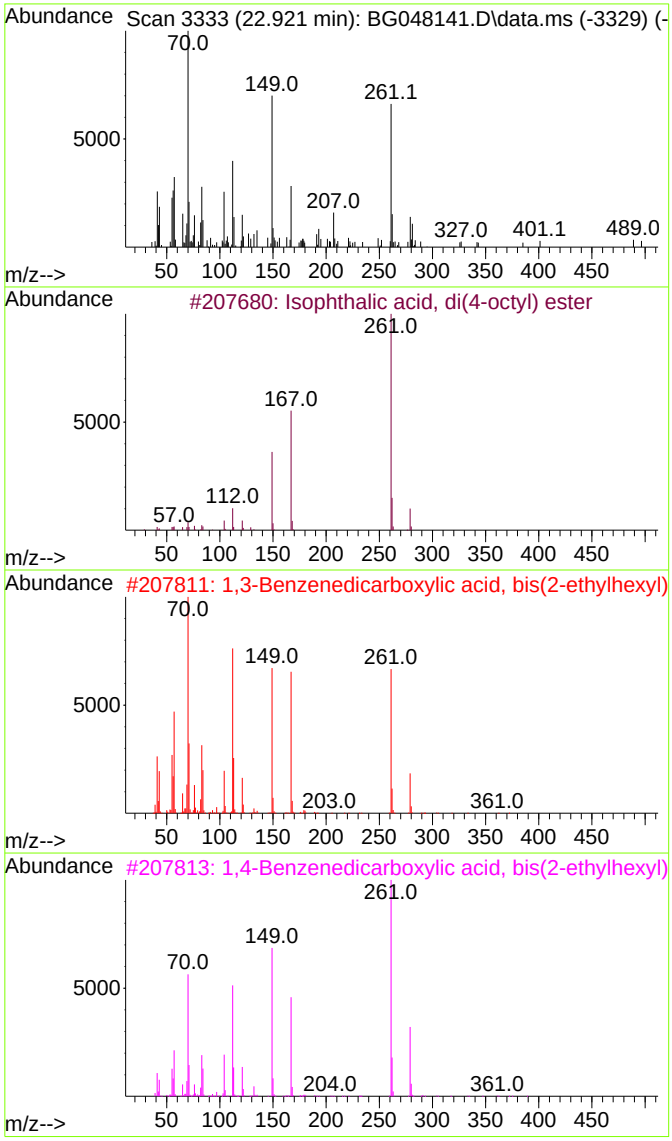
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

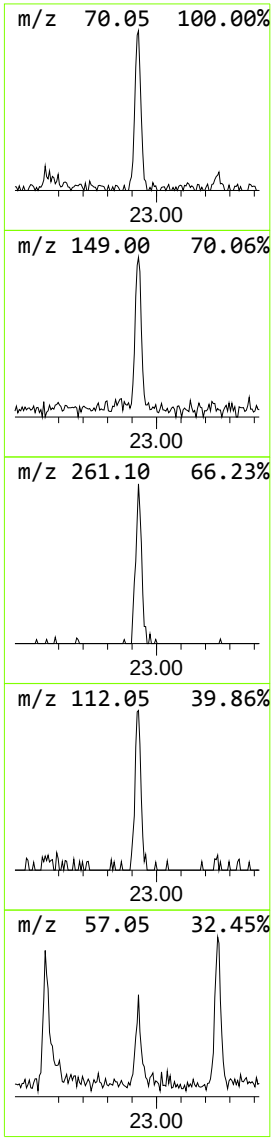
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Isophthalic acid, di(4-octy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.921	2.47 ng	123299	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	58
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
3	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
5	Terephthalic acid, 4-chloro-3-me...	402	C23H27ClO4	1000323-70-4	27





Tentatively Identified Compound (LSC) summary

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Operator : CG/JU
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Instrument : BNA_G
ClientSampleId : NAB-210209-MNT-BP25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
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
unknown9.419	9.419	7.2	ng	99055	1	8.103	275703	20.0
Ethanol, 2-(2-b...	10.676	2.9	ng	54328	2	10.917	377650	20.0
Nonanoic acid	11.704	9.2	ng	174510	2	10.917	377650	20.0
Undecanoic acid	15.130	3.0	ng	93031	3	14.724	626643	20.0
n-Hexadecanoic ...	18.355	25.2	ng	1061640	4	17.468	843203	20.0
Octadecanoic acid	19.613	13.5	ng	675540	5	21.734	998064	20.0
Cyclohexadecane	21.370	12.0	ng	596671	5	21.734	998064	20.0
Isophthalic aci...	22.921	2.5	ng	123299	5	21.734	998064	20.0