LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

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-BG101818.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	5.543	376	384	397	rBV	1280646	2084278	3.85%	1.986%
2	5.755	411	420	431	rVB2	368248	891624	1.65%	0.850%
3	6.272	481	508	511	rBV2	9431754	54130881	100.00%	51.584%
4	7.253	663	675	687	rBV2	384085	838655	1.55%	0.799%
5	7.641	733	741	753	rVB	980655	1772209	3.27%	1.689%
6	8.428	869	875	890	rVB	811233	1532096	2.83%	1.460%
7	9.280	969	1020	1030	rBV2	2700429	18561547	34.29%	17.688%
8	10.925	1293	1300	1308	rVB	344278	642387	1.19%	0.612%
9	12.189	1507	1515	1523	rBV2	316478	867824	1.60%	0.827%
10	13.364	1708	1715	1721	rBV	1866041	2998407	5.54%	2.857%
11	13.675	1762	1768	1772	rBV	1327198	2009952	3.71%	1.915%
12	14.739	1943	1949	1956	rVB2	529915	908087	1.68%	0.865%
13	15.150	2013	2019	2026	rBV3	545149	991822	1.83%	0.945%
14	16.237	2196	2204	2210	rBV2	2353777	4305490	7.95%	4.103%
15	17.488	2412	2417	2422	rBV	623863	924703	1.71%	0.881%
16	18.299	2550	2555	2560	rBV	1467434	2074575	3.83%	1.977%
17	18.352	2560	2564	2577	rVB	798850	1135885	2.10%	1.082%
18	19.956	2833	2837	2848	rBV	1137069	1465098	2.71%	1.396%
19	20.085	2854	2859	2867	rVB	2617775	3468157	6.41%	3.305%
20	21.348	3070	3074	3088	rVB2	537165	1094255	2.02%	1.043%
21	21.771	3140	3146	3155	rVB	602057	1042309	1.93%	0.993%
22	25.109	3703	3714	3727	rVB2	354401	1196138	2.21%	1.140%

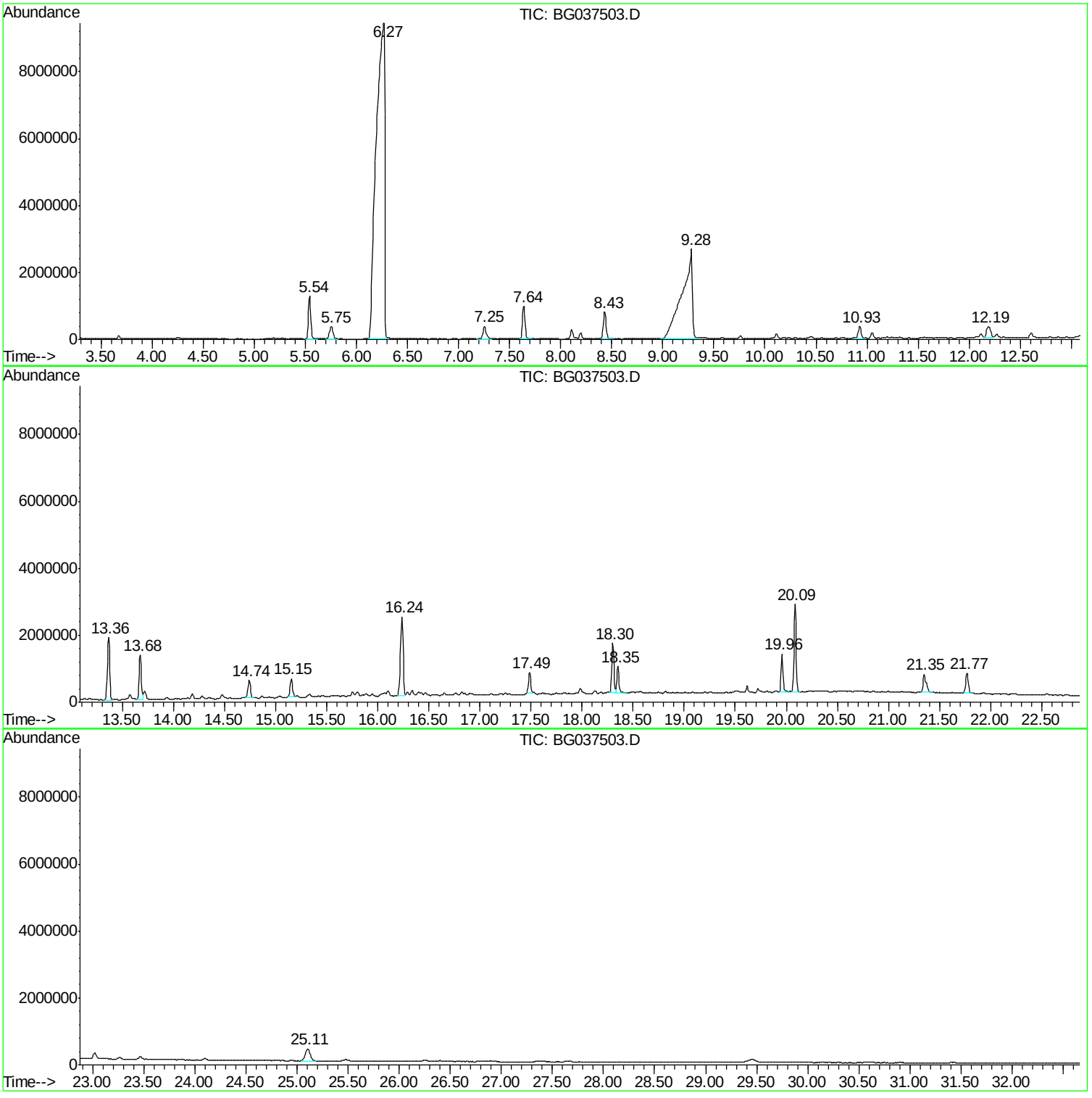
Sum of corrected areas: 104936379

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

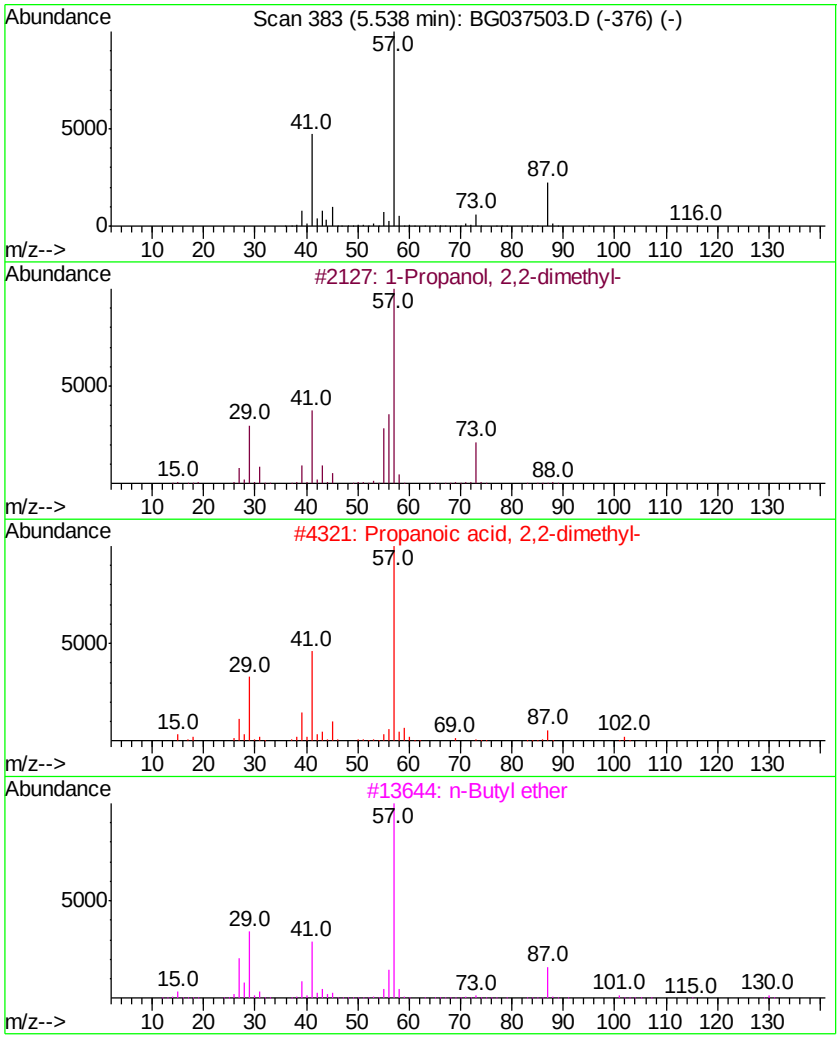
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

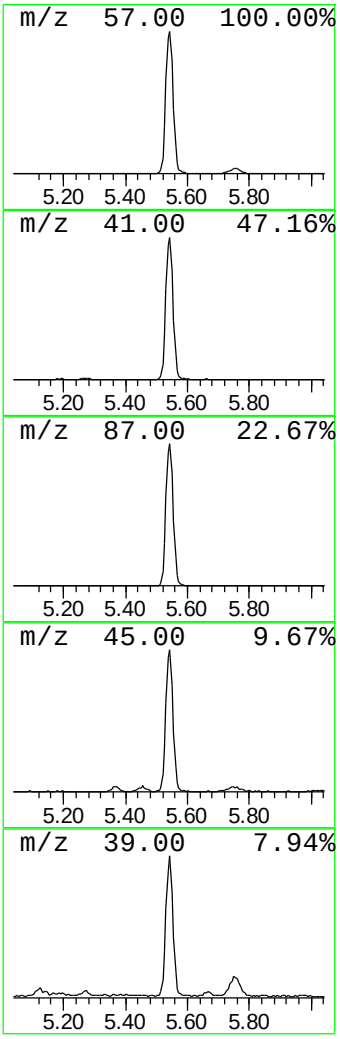
****

Peak Number 1 unknown5.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	27.21 ng	2084280	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
3	n-Butyl ether	130	C8H18O	000142-96-1	36
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
5	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	28





Library Search Compound Report

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Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

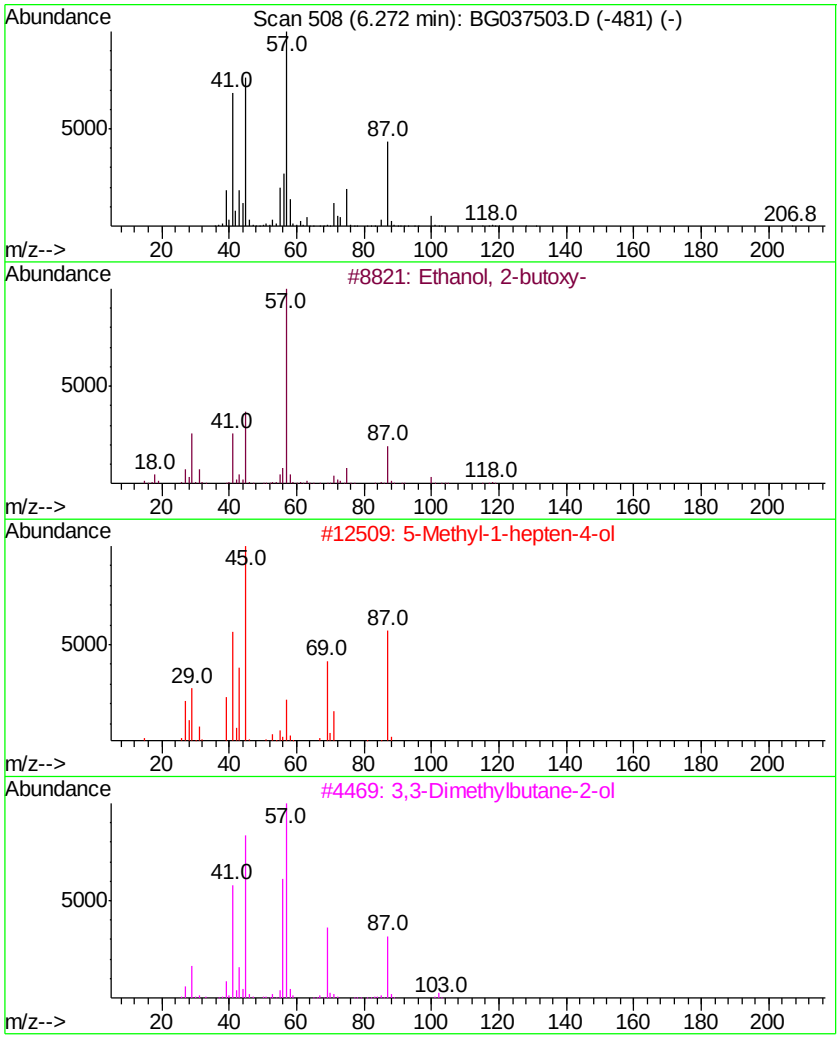
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

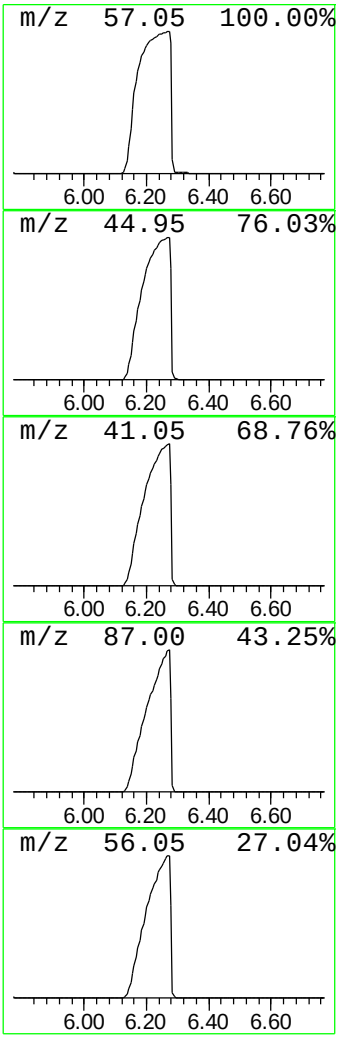
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	706.63 ng	54130900	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2	5-Methyl-1-hepten-4-ol	128	C8H16O	099328-46-8	50
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
5	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	37





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

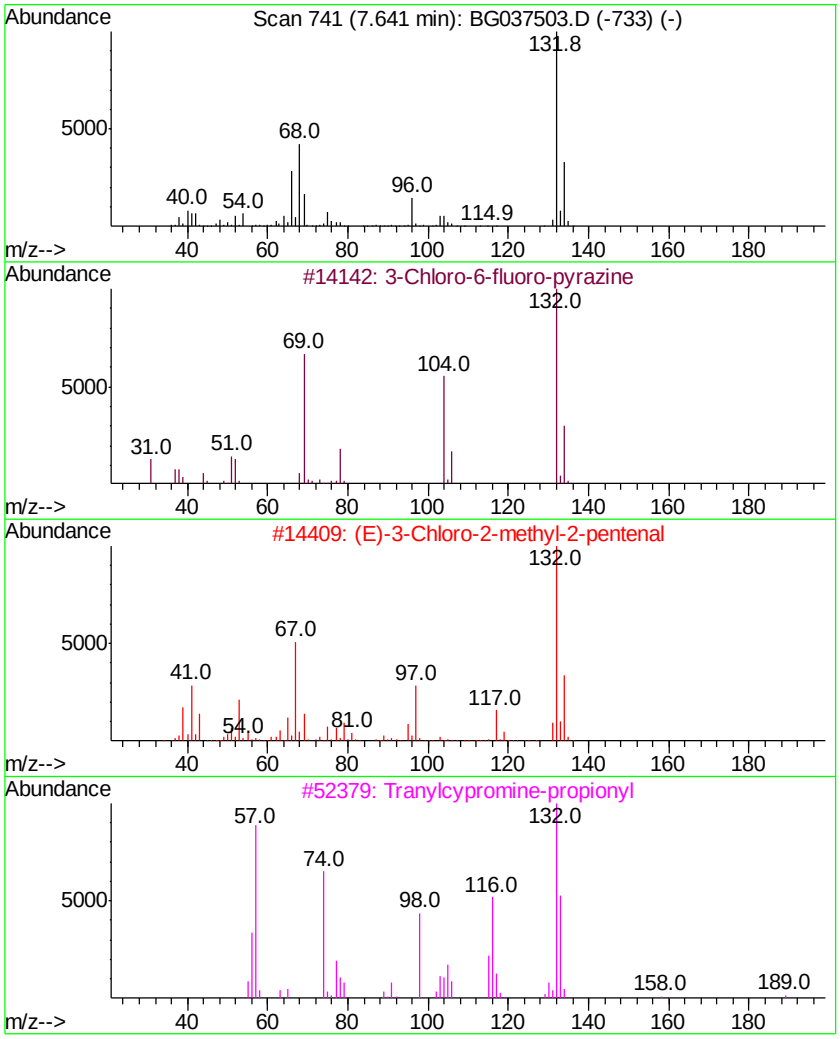
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

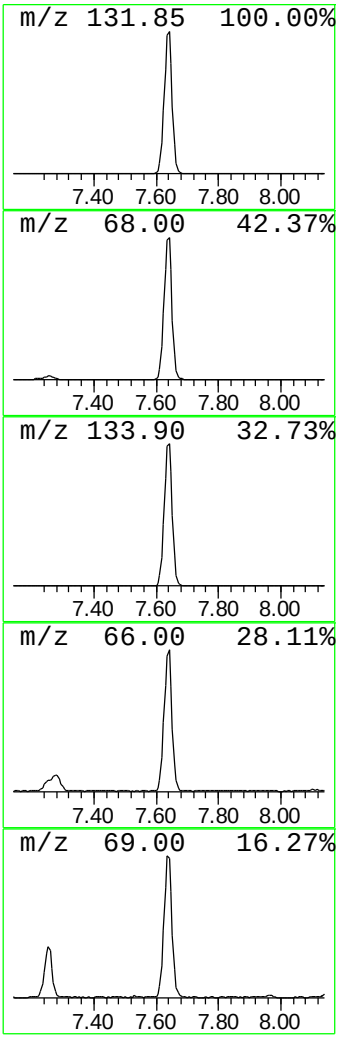
****

Peak Number 3 unknown7.64 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	23.13 ng	1772210	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

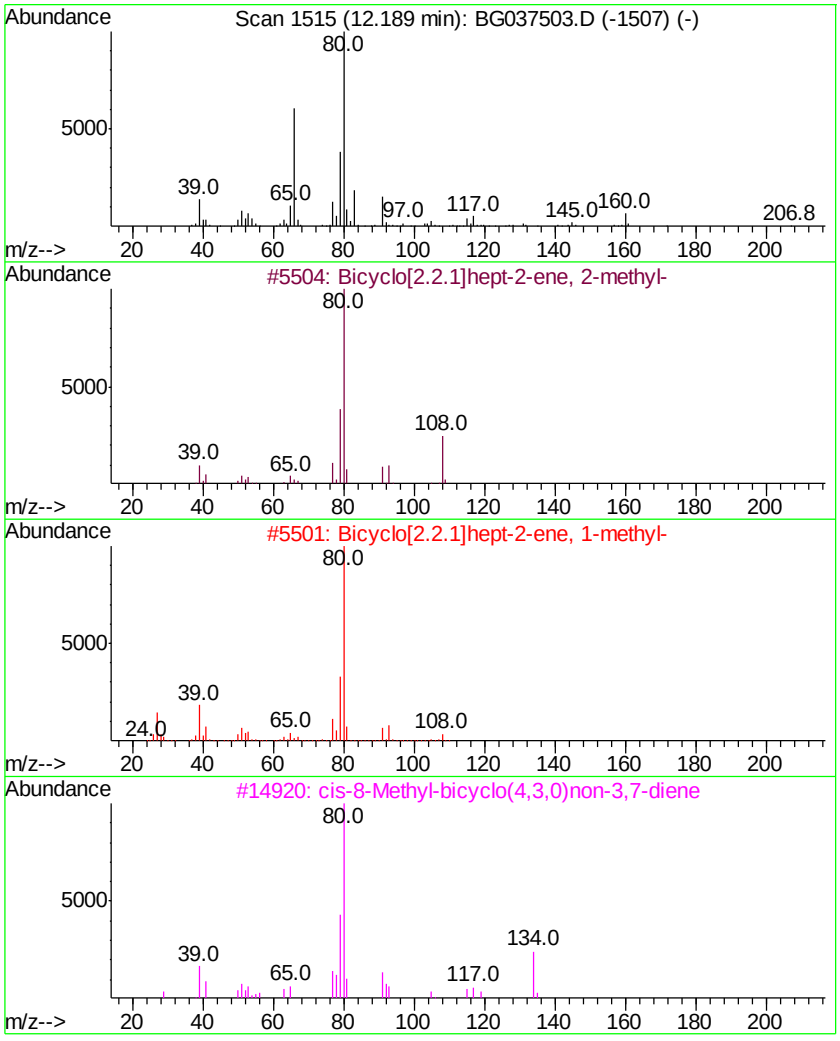
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

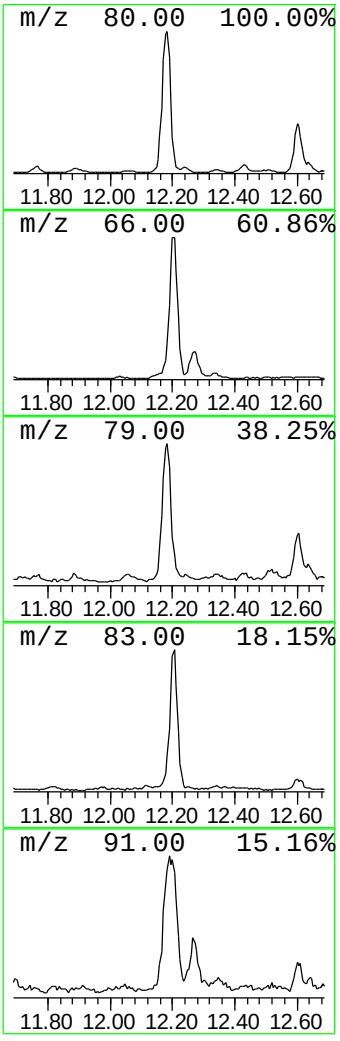
****

Peak Number 5 Bicyclo[2.2.1]hept-2-ene, 2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	27.02 ng	867824	Naphthalene-d8	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]hept-2-ene, 2-methyl-	108	C8H12	000694-92-8	50
2	Bicyclo[2.2.1]hept-2-ene, 1-methyl-	108	C8H12	000822-73-1	50
3	cis-8-Methyl-bicyclo(4,3,0)non-3...	134	C10H14	1000144-50-6	50
4	3-Oxabicyclo[3.3.0]octan-2-one, ...	138	C8H10O2	1000152-82-0	50
5	Biphenylene, 1,2,4a,4b,7,8,8a,8b...	160	C12H16	062357-80-6	47





Library Search Compound Report

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Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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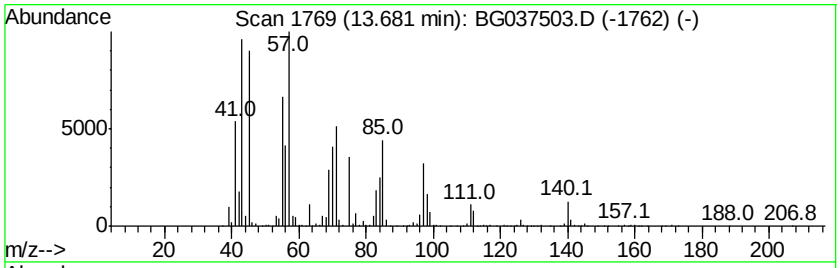
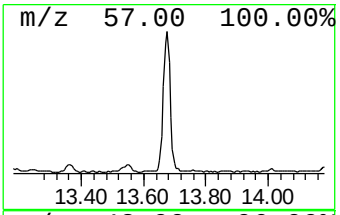
****

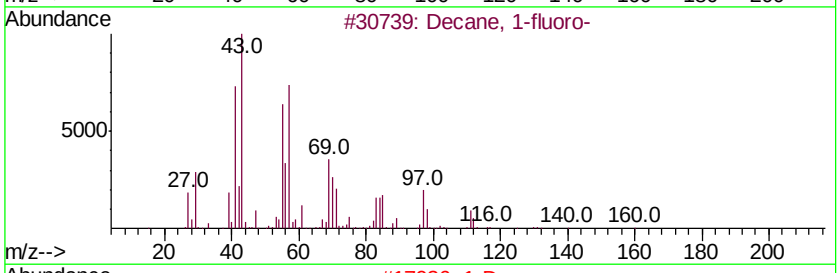
Peak Number 6 unknown13.68 Concentration Rank 3

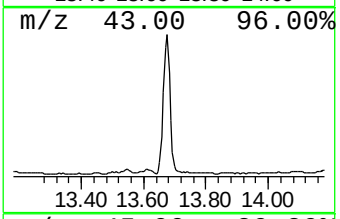
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	44.27 ng	2009950	Acenaphthene-d10	14.74

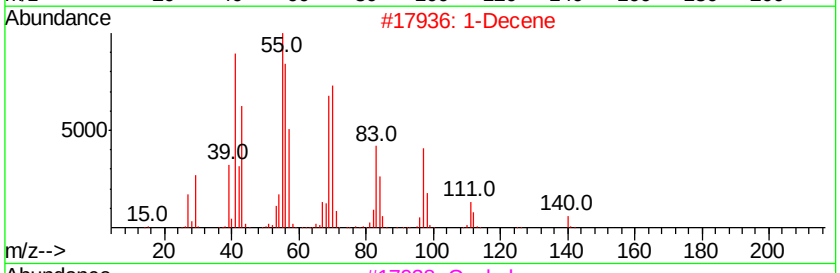
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 1-fluoro-	160	C10H21F	000334-56-5	46
2	1-Decene	140	C10H20	000872-05-9	46
3	Cyclodecane	140	C10H20	000293-96-9	41
4	Decane, 3-chloro-	176	C10H21Cl	001002-11-5	35
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	35

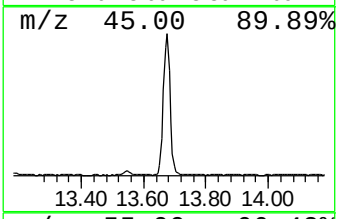


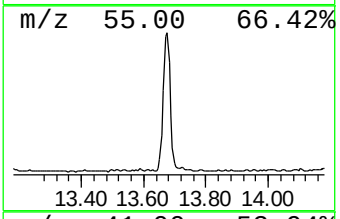


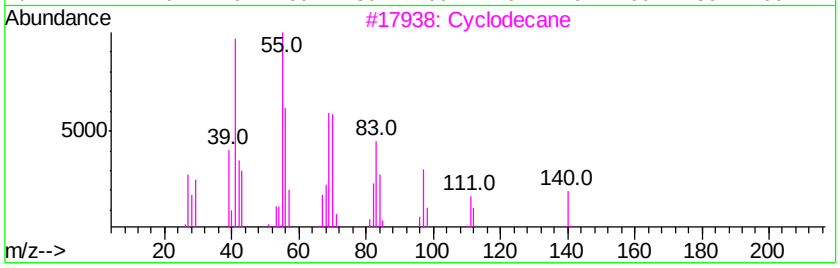


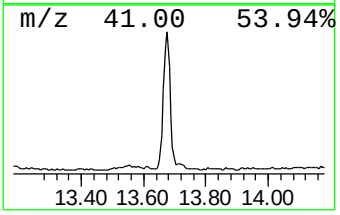












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
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ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

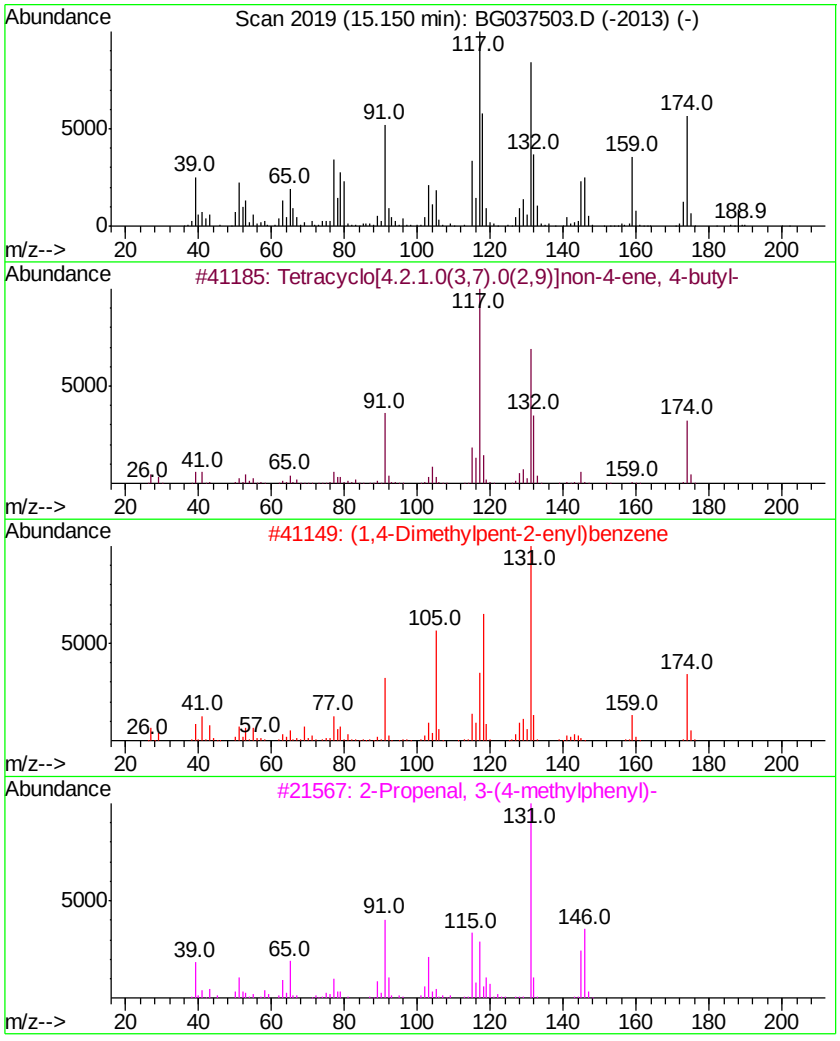
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

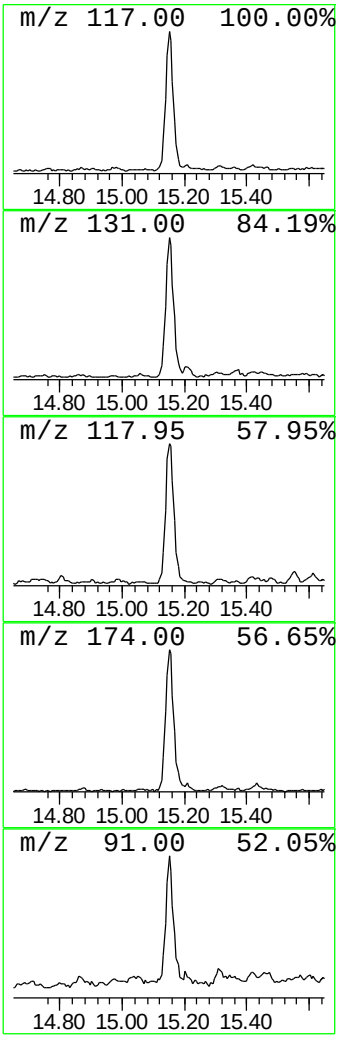
****

Peak Number 7 Tetracyclo[4.2.1.0(3,7).0(2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	21.84 ng	991822	Acenaphthene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[4.2.1.0(3,7).0(2,9)]n...	174	C13H18	1000164-31-2	64
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	49
3	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	46
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	46
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	46





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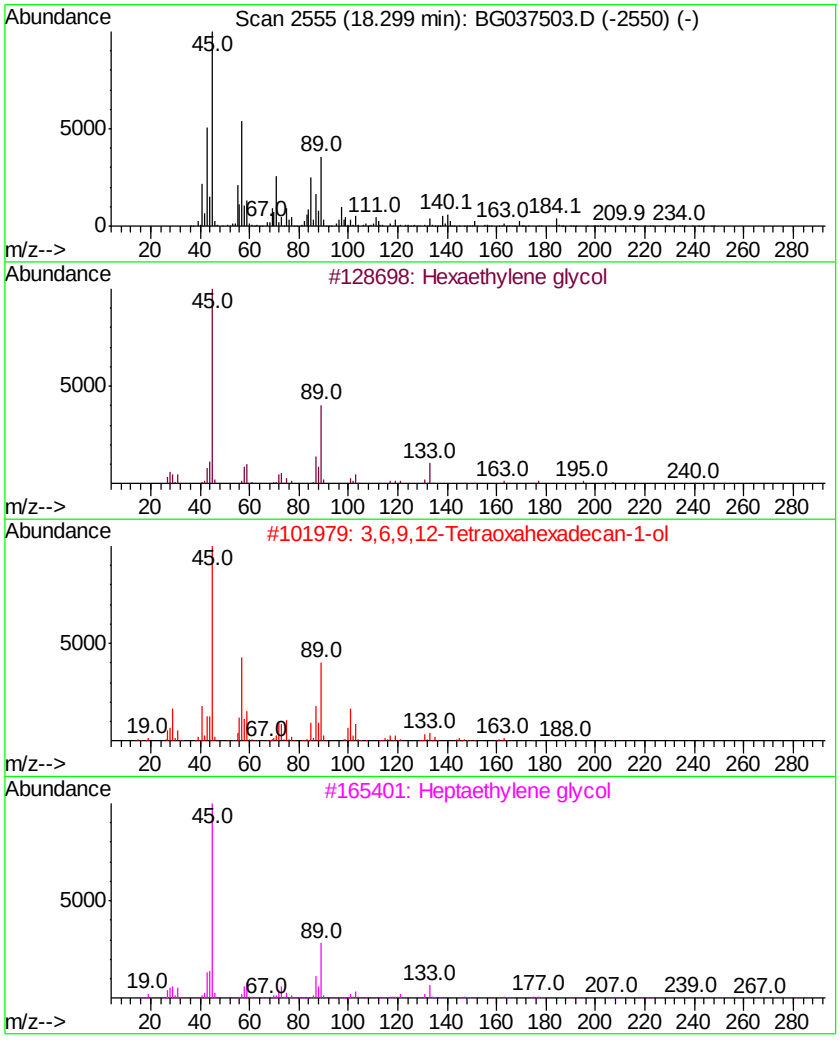
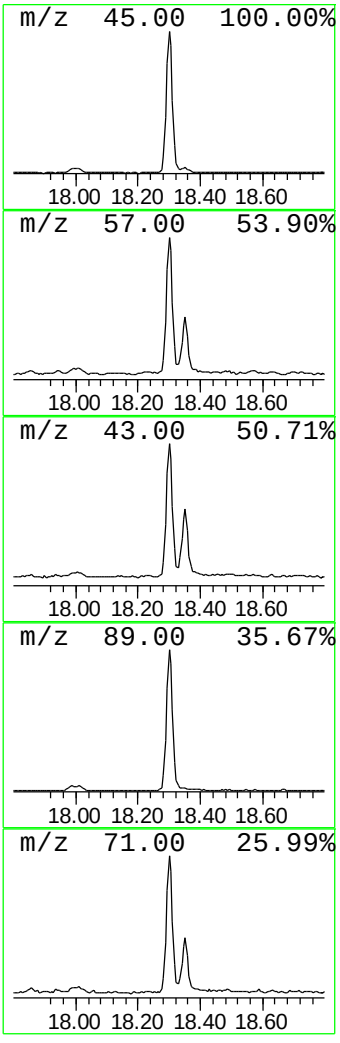
****

Peak Number 8 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	44.87 ng	2074580	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	52
2	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	52
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	50
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
5	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	50





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Misc :
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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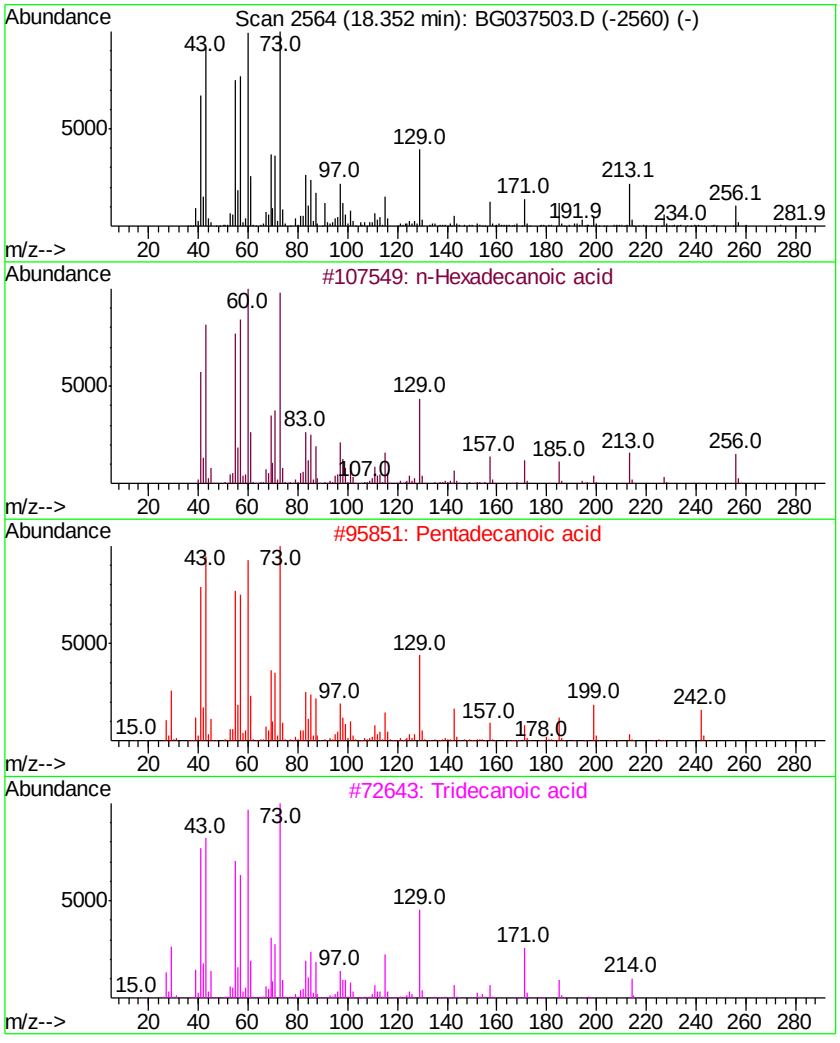
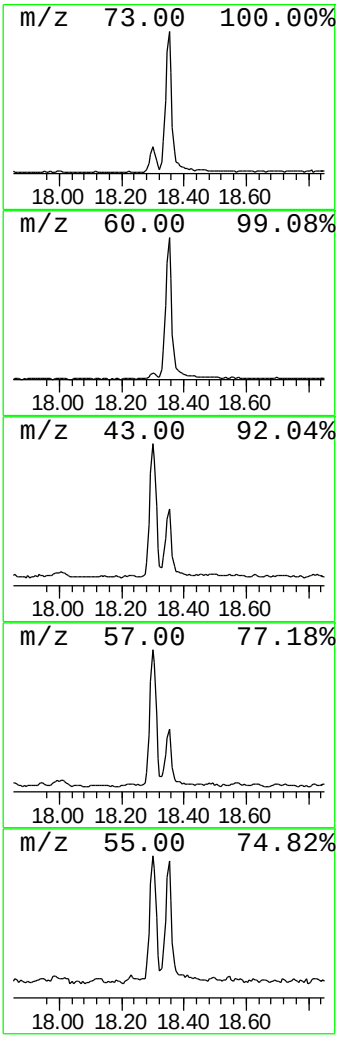
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	24.57 ng	1135890	Phenanthrene-d10	17.49

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	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

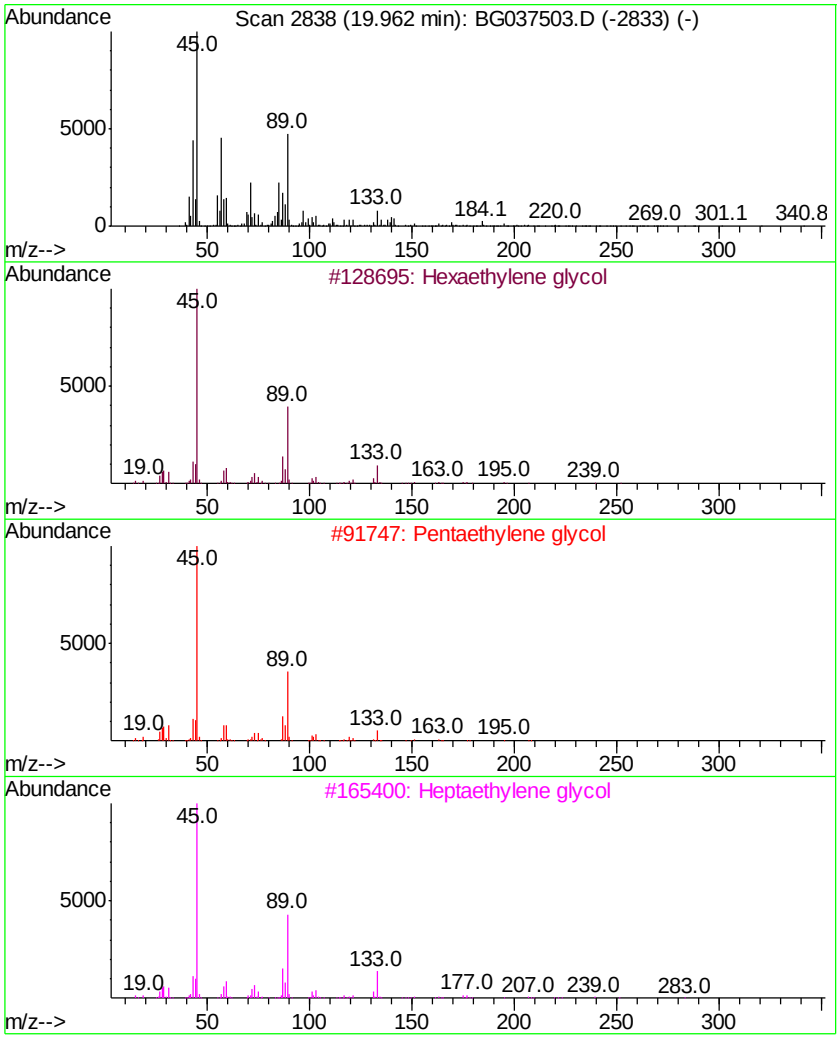
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

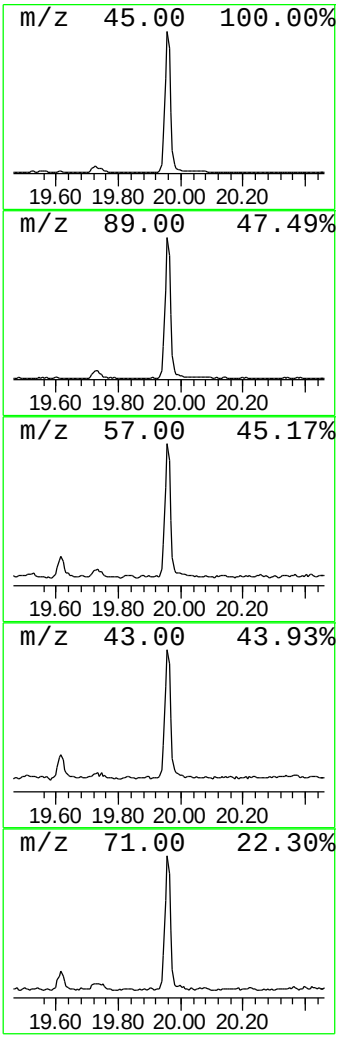
****

Peak Number 10 Heptaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.96	28.11 ng	1465100	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	68
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	68
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	68
4	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	59
5	Triethylene glycol	150	C6H14O4	000112-27-6	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

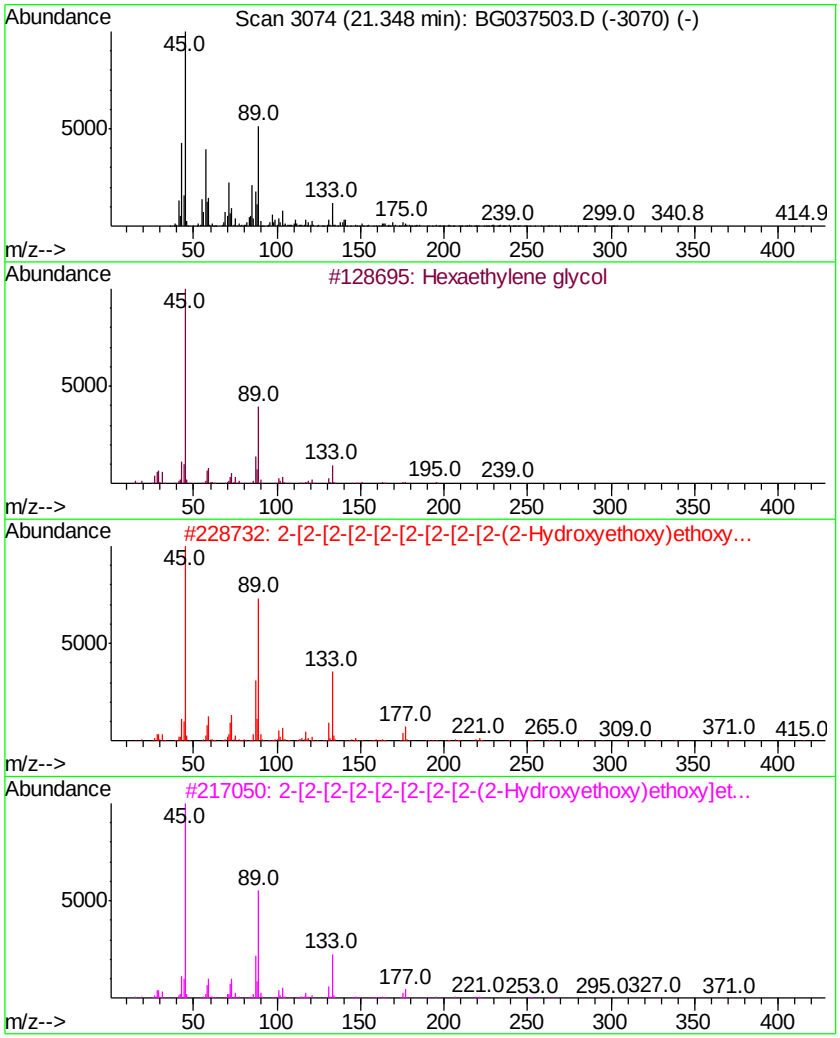
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

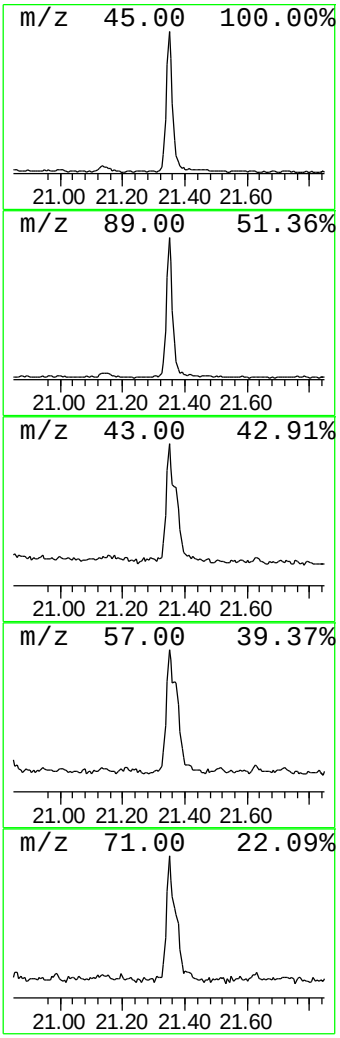
****

Peak Number 11 Hexaethylene glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	21.00 ng	1094260	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	74
2	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	72
3	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	72
4	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	72
5	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102318\
Data File : BG037503.D
Acq On : 24 Oct 2018 9:37
Operator : JU/SJ
Sample : J5604-08
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
unknown5.54	5.54	27.2	ng	2084280	1	8.11	1532100	20.0
Ethanol, 2-butoxy-	6.27	706.6	ng	54130900	1	8.11	1532100	20.0
unknown7.64	7.64	23.1	ng	1772210	1	8.11	1532100	20.0
Bicyclo[2.2.1]hep...	12.19	27.0	ng	867824	2	10.93	642387	20.0
unknown13.68	13.68	44.3	ng	2009950	3	14.74	908087	20.0
Tetracyclo[4.2.1....	15.15	21.8	ng	991822	3	14.74	908087	20.0
3,6,9,12-Tetraoxa...	18.30	44.9	ng	2074580	4	17.49	924703	20.0
n-Hexadecanoic acid	18.35	24.6	ng	1135890	4	17.49	924703	20.0
Heptaethylene glycol	19.96	28.1	ng	1465100	5	21.77	1042310	20.0
Hexaethylene glycol	21.35	21.0	ng	1094260	5	21.77	1042310	20.0