LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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	55349	87436	5.15%	0.993%
2	4.533	240	246	253	rBV	105603	166213	9.79%	1.888%
3	5.138	343	349	359	rBV	150236	243951	14.36%	2.772%
4	5.602	422	428	441	rBV	313058	536452	31.59%	6.095%
5	6.108	509	514	520	rBV2	15875	26531	1.56%	0.301%
6	7.206	694	701	713	rBV	348731	641663	37.78%	7.290%
7	7.588	758	766	775	rBV	324139	587649	34.60%	6.676%
8	8.058	840	846	852	rBV	76137	131553	7.75%	1.495%
9	8.381	893	901	910	rBV	290480	520745	30.66%	5.916%
10	9.233	1038	1046	1056	rBV	236592	444518	26.17%	5.050%
11	10.878	1318	1326	1334	rBV	103732	198870	11.71%	2.259%
12	13.317	1734	1741	1749	rBV	744878	1176579	69.28%	13.367%
13	13.828	1822	1828	1833	rBV9	8369	19204	1.13%	0.218%
14	13.957	1846	1850	1854	rBV6	10757	19690	1.16%	0.224%
15	14.139	1877	1881	1885	rVB2	21649	32032	1.89%	0.364%
16	14.192	1887	1890	1894	rVB5	33801	47732	2.81%	0.542%
17	14.510	1940	1944	1947	rVB5	25780	42620	2.51%	0.484%
18	14.698	1971	1976	1982	rVB2	185341	319864	18.83%	3.634%
19	16.190	2225	2230	2236	rBV2	424608	645453	38.01%	7.333%
20	18.440	2611	2613	2614	rBV	153362	109015	6.42%	1.239%
21	20.050	2882	2887	2893	rVB	1258716	1698322	100.00%	19.295%
22	21.719	3165	3171	3180	rVB2	237918	426182	25.09%	4.842%
23	25.015	3723	3732	3743	rVB3	148407	426529	25.11%	4.846%
24	27.547	4153	4163	4164	rBV2	48906	101399	5.97%	1.152%
25	28.981	4392	4407	4421	rBV5	33553	151826	8.94%	1.725%

Sum of corrected areas: 8802028

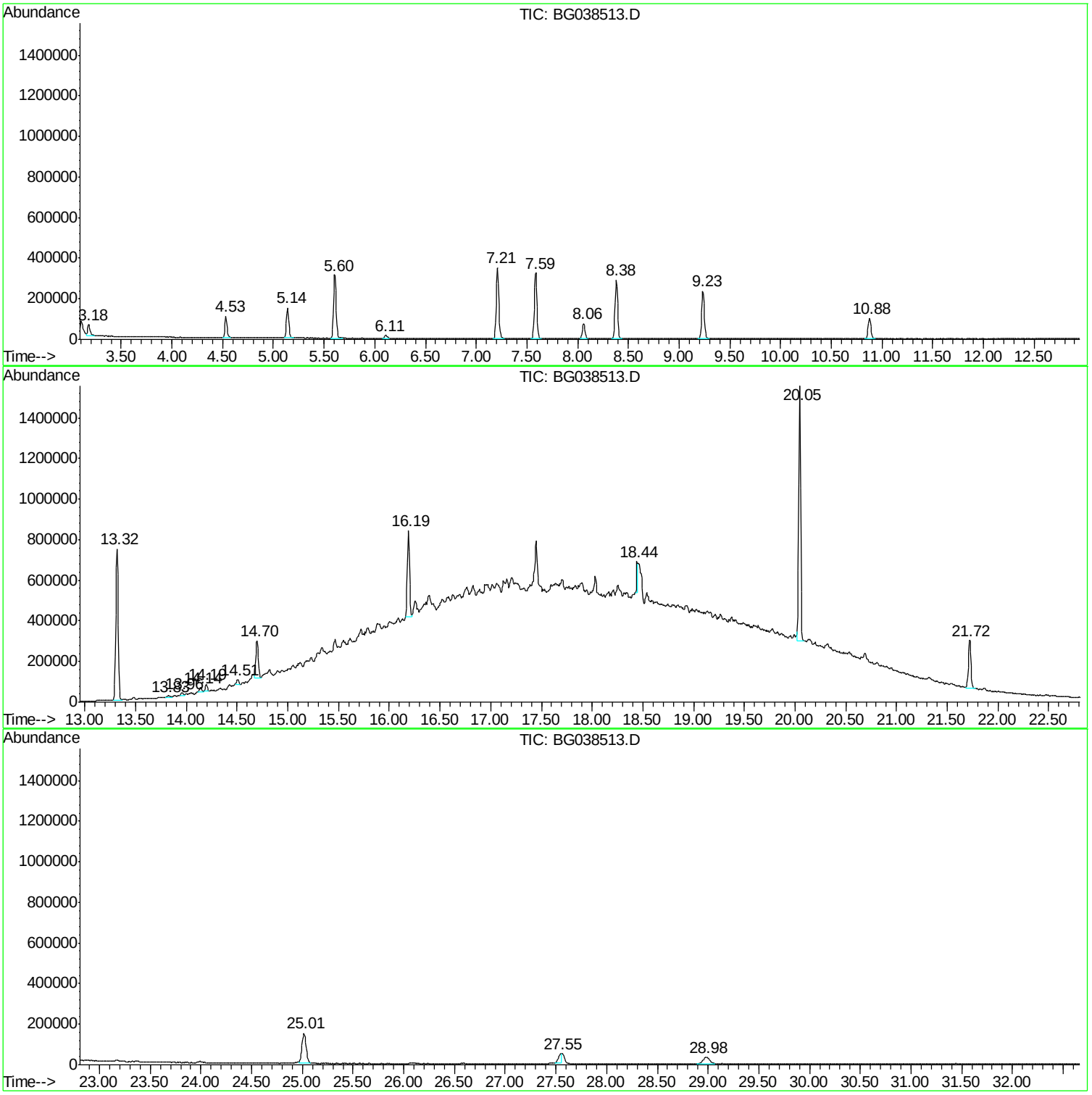
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

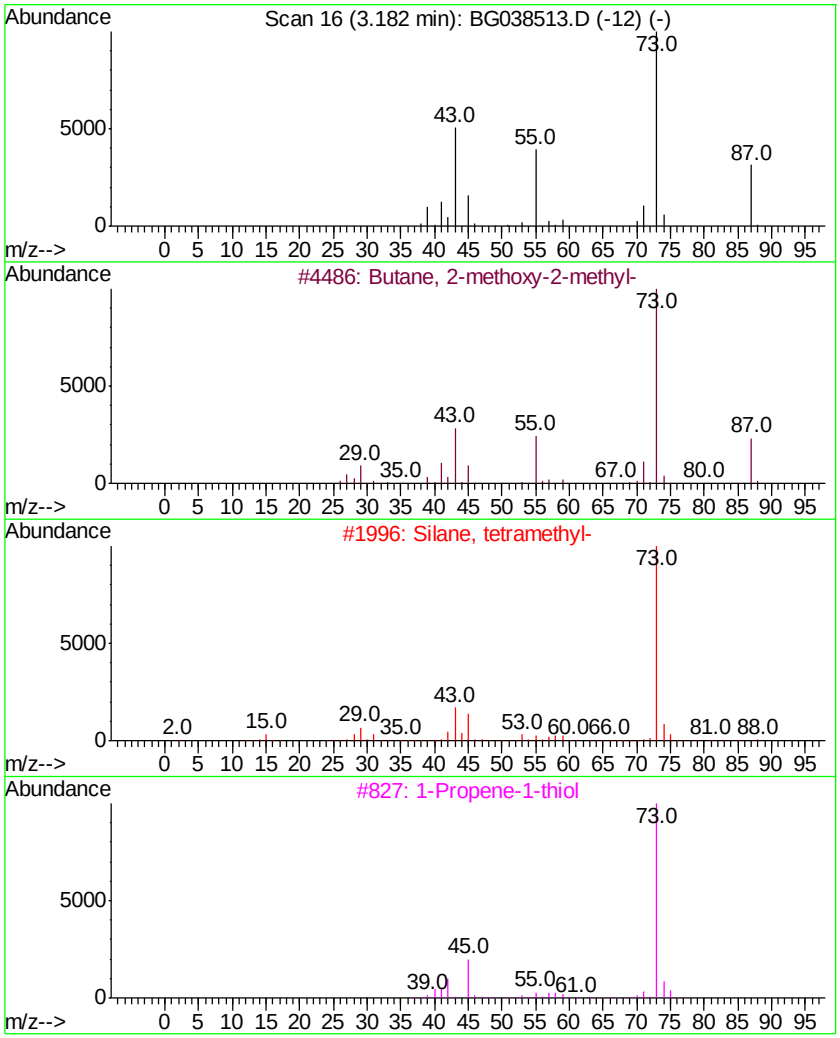
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

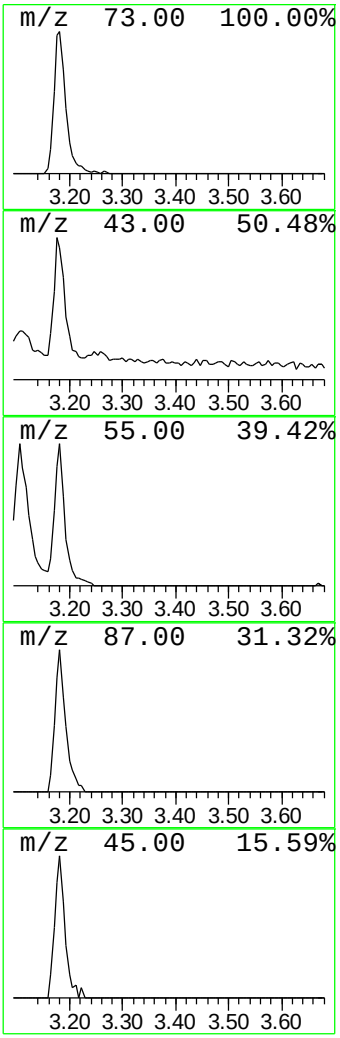
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	13.29 ng	87436	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	64
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

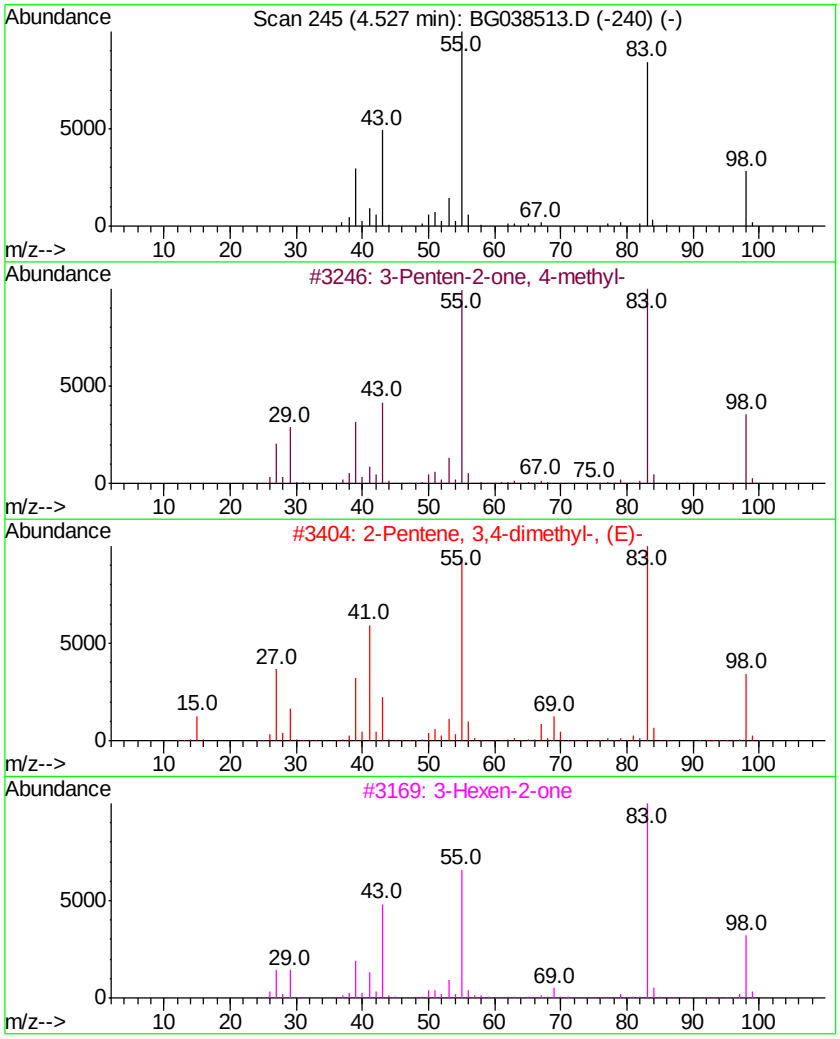
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

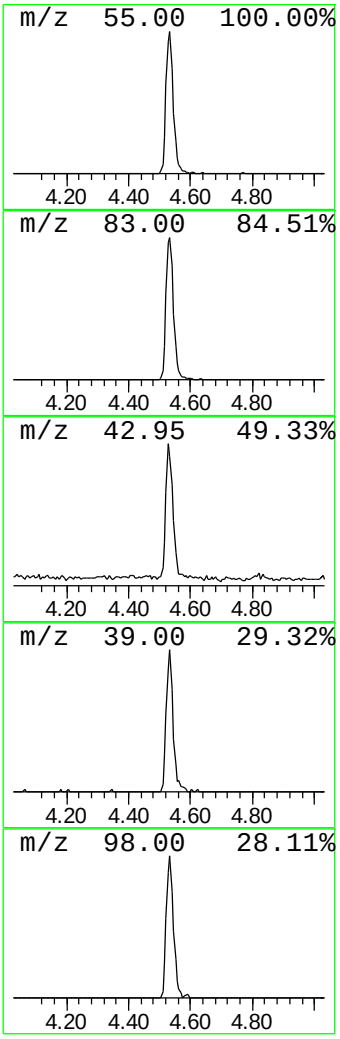
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	25.27 ng	166213	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	80
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

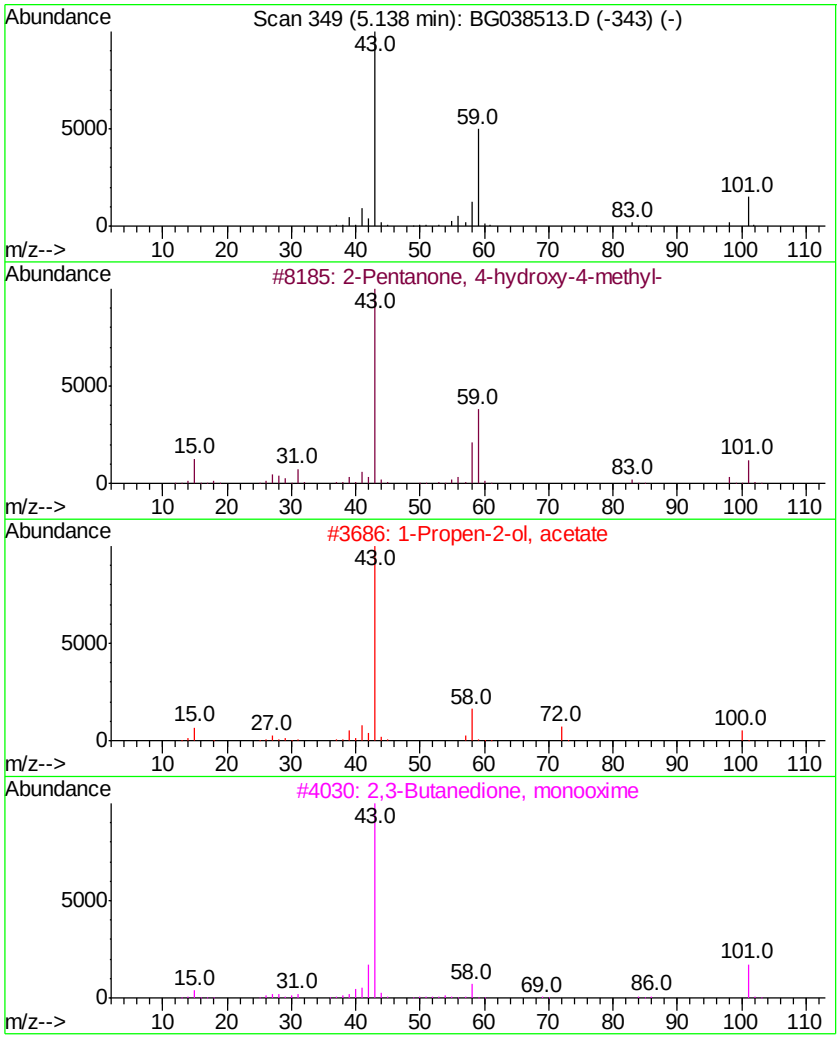
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

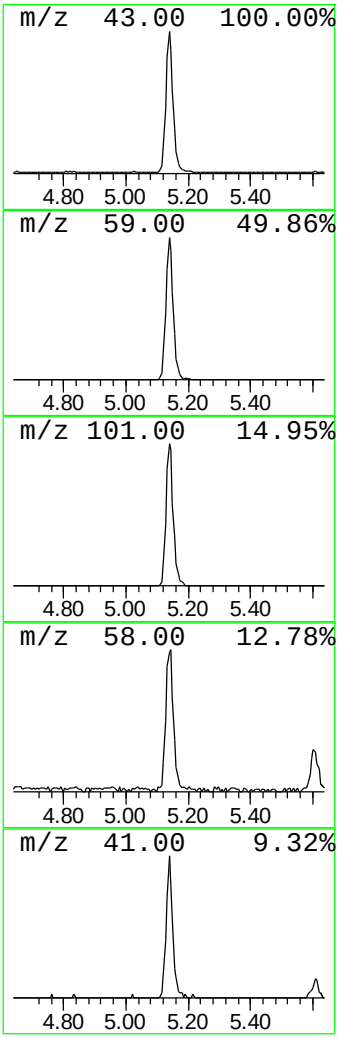
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	37.09 ng	243951	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	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	8





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

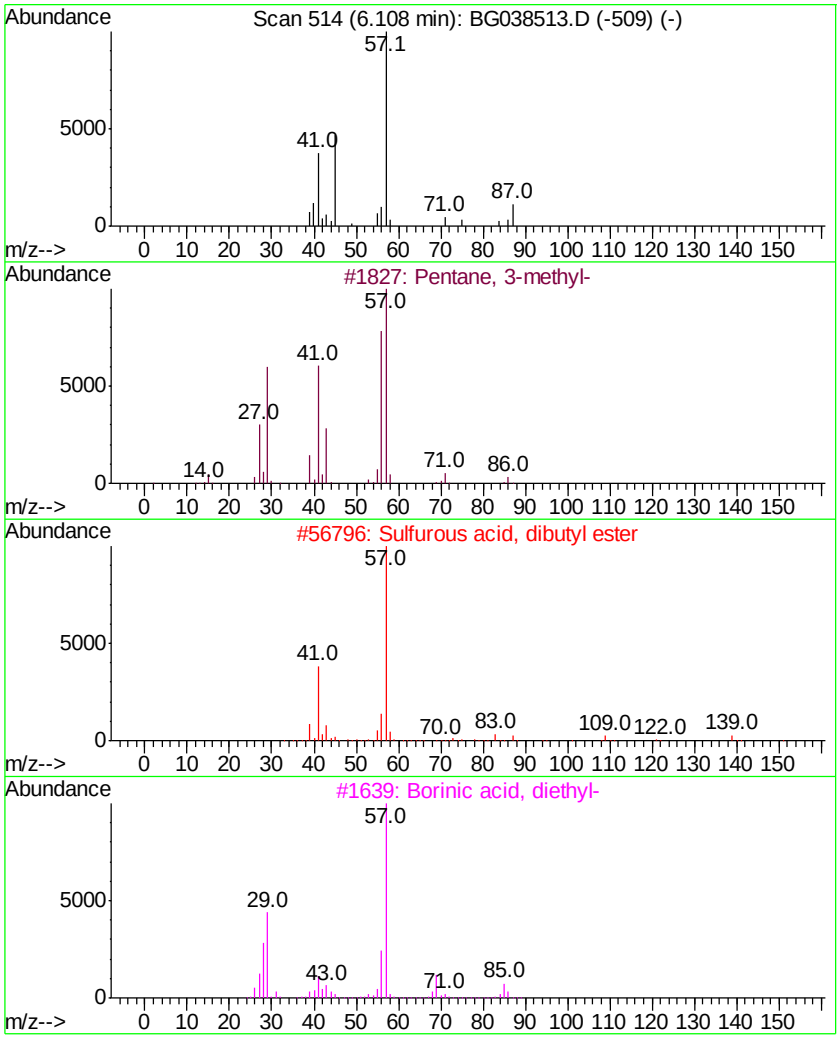
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

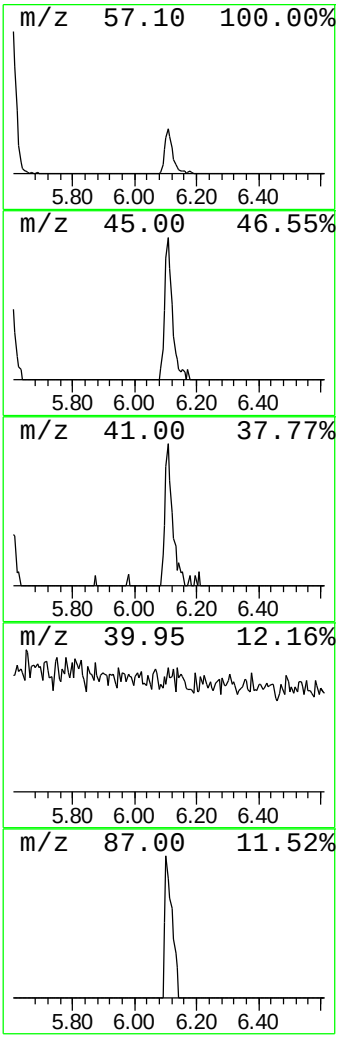
****

Peak Number 4 unknown6.11 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.11	4.03 ng	26531	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	25
2	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	16
3	Borinic acid, diethyl-	86	C4H11BO	004426-31-7	10
4	1-Penten-3-ol	86	C5H10O	000616-25-1	9
5	2-Methoxyethyl 2-methylbutanoate	160	C8H16O3	1000366-96-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

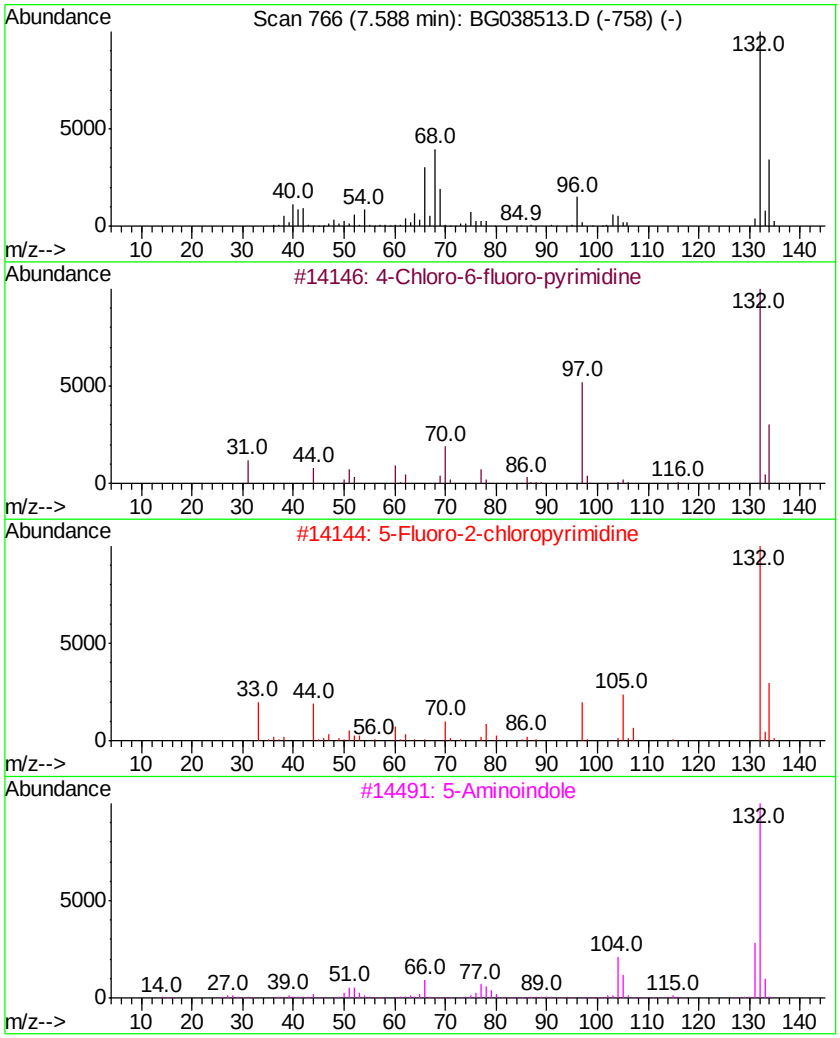
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

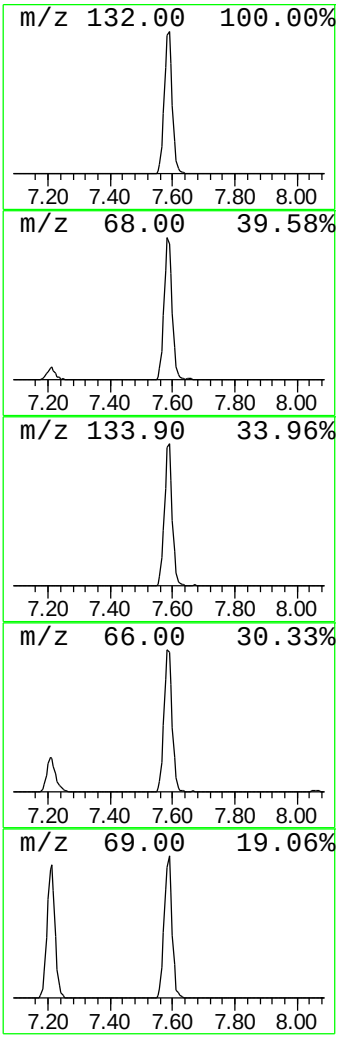
****

Peak Number 5 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	89.34 ng	587649	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

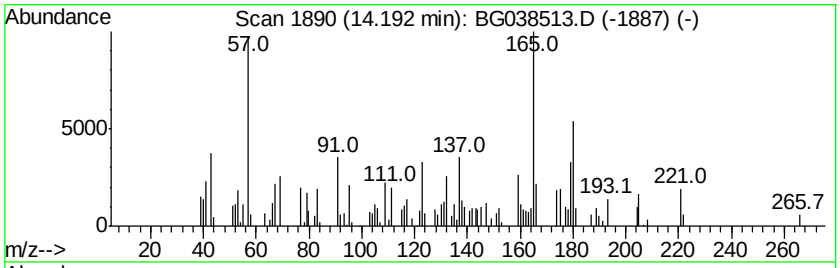
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

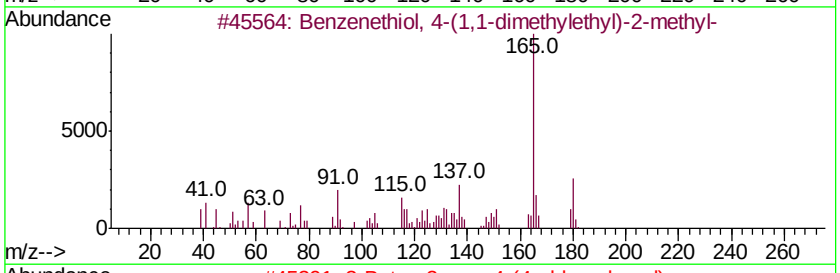
****

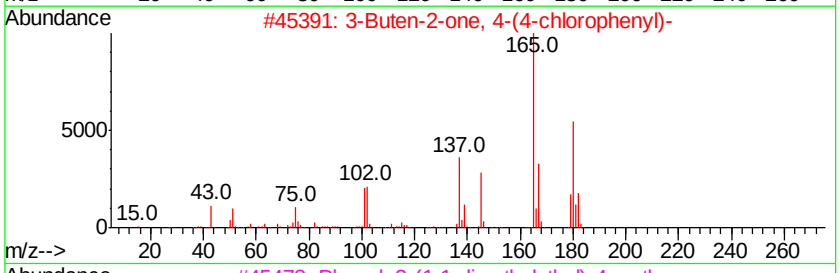
Peak Number 7 Benzenethiol, 4-(1,1-dimeth... Concentration Rank 10

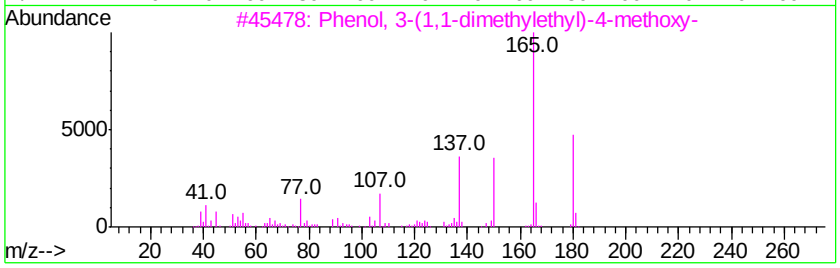
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.98 ng	47732	Acenaphthene-d10	14.70

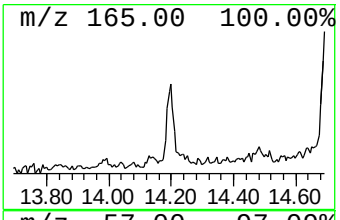
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	52
2	3-Buten-2-one, 4-(4-chlorophenyl)-	180	C10H9ClO	003160-40-5	46
3	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	46
4	9H-Fluorene, 1-methyl-	180	C14H12	001730-37-6	43
5	Silane, trimethyl(4-methylphenoxy)-	180	C10H16OSi	017902-32-8	43

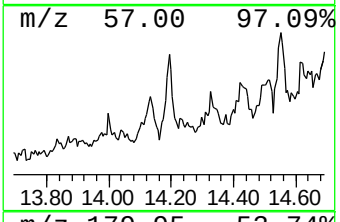


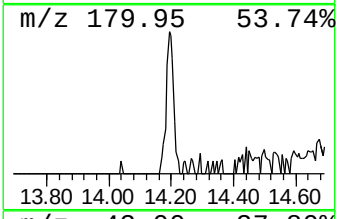


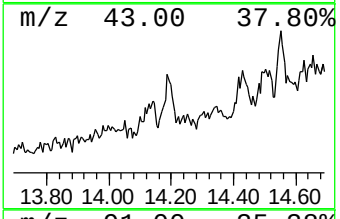


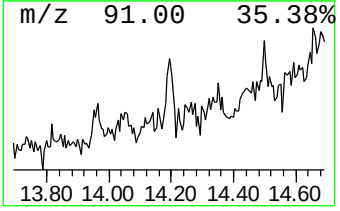












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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

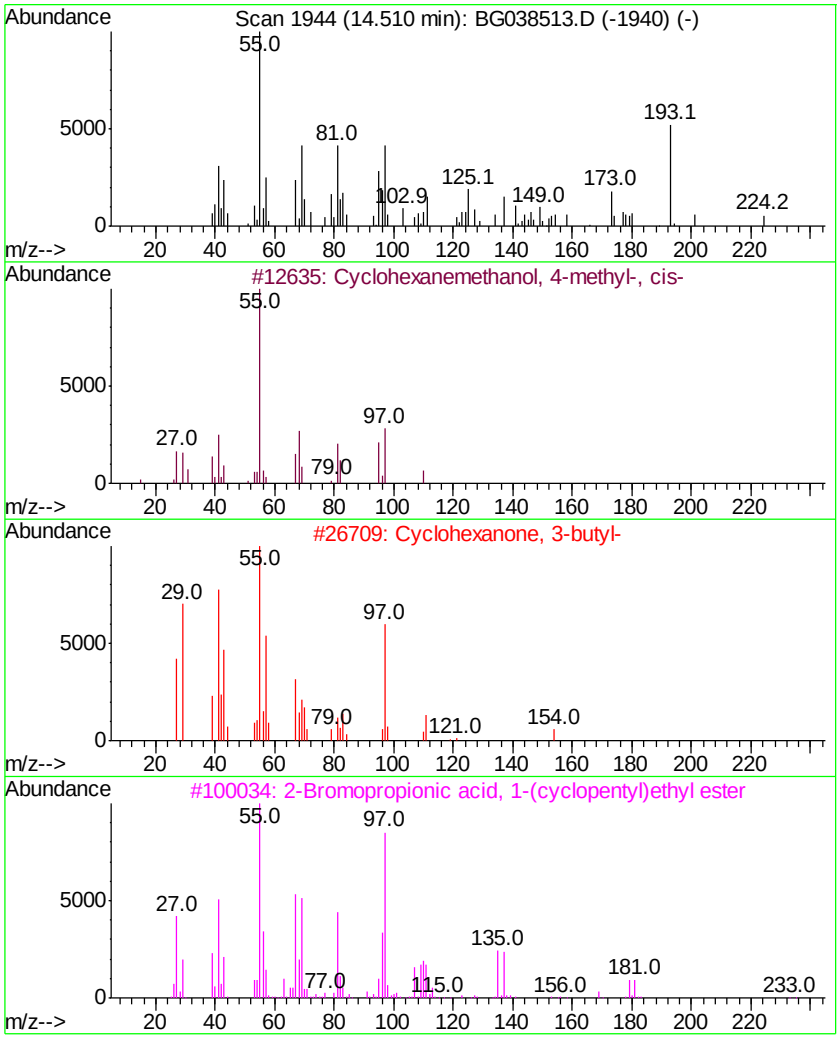
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

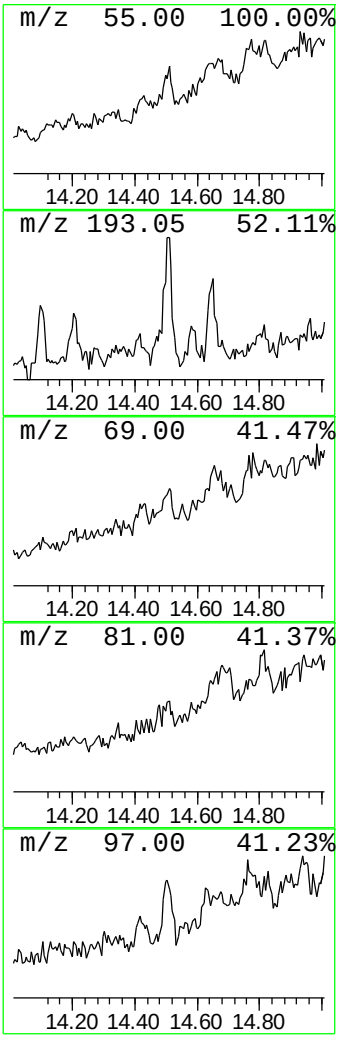
****

Peak Number 8 unknown14.51 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.66 ng	42620	Acenaphthene-d10	14.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	22
2	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	18
3	2-Bromopropionic acid, 1-(cyclop...	248	C10H17BrO2	1000293-39-1	16
4	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	14
5	1,10-Hexadecanediol	258	C16H34O2	039516-54-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
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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-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

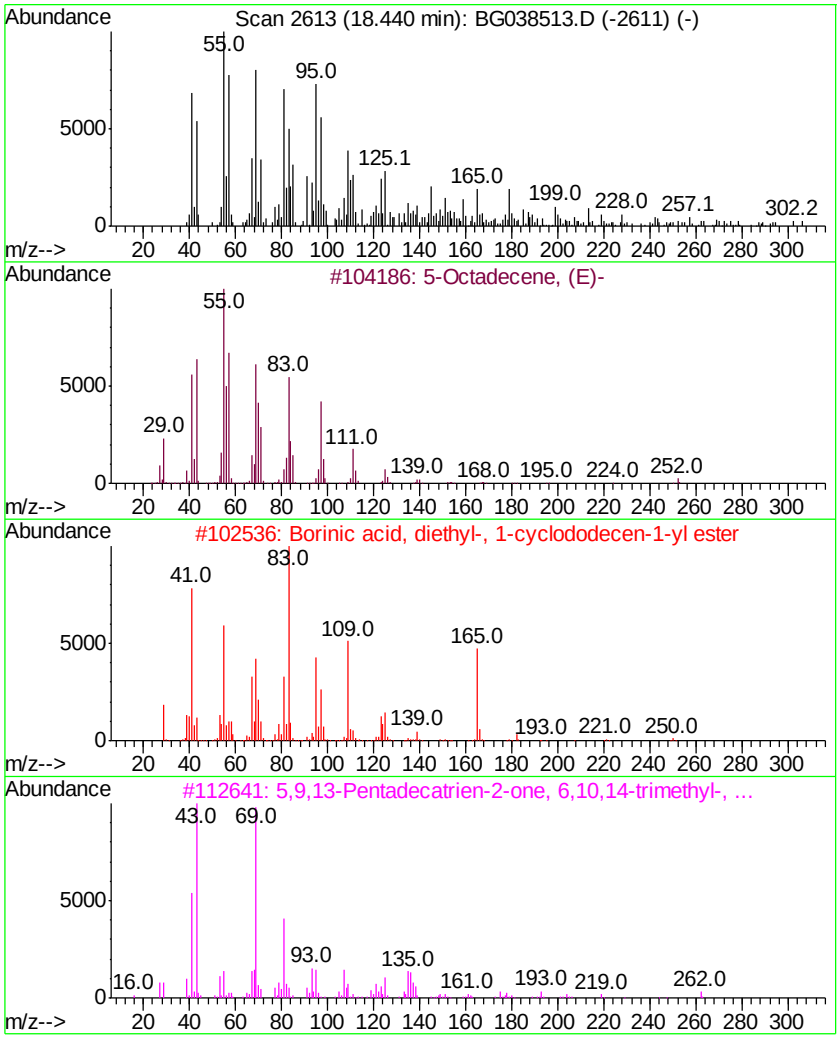
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

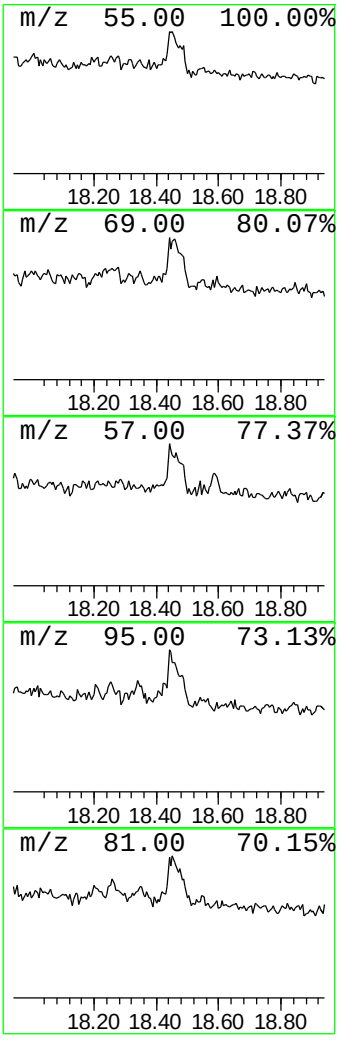
****

Peak Number 9 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	20.00 ng	109015	Phenanthrene-d10	17.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	51
2	Borinic acid, diethyl-, 1-cyclod...	250	C16H31BO	061142-73-2	41
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	35
4	3,8-Nonadien-2-one, (E)-	138	C9H14O	055282-90-1	25
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	25





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Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

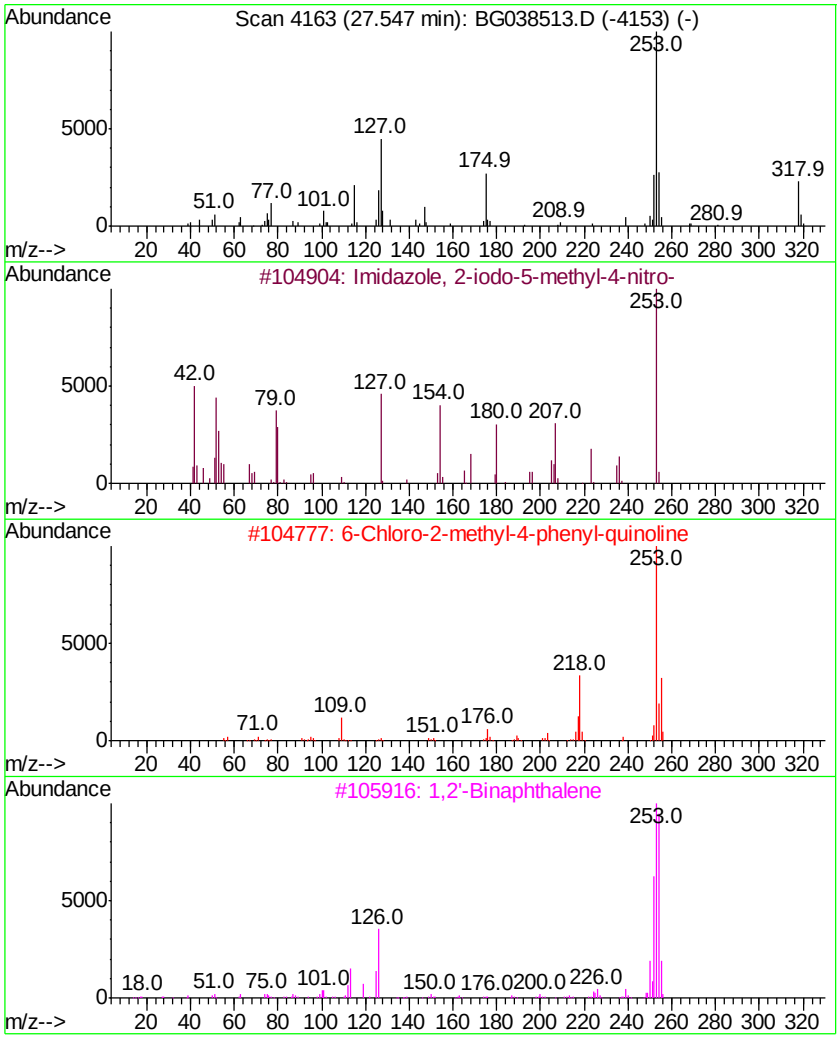
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

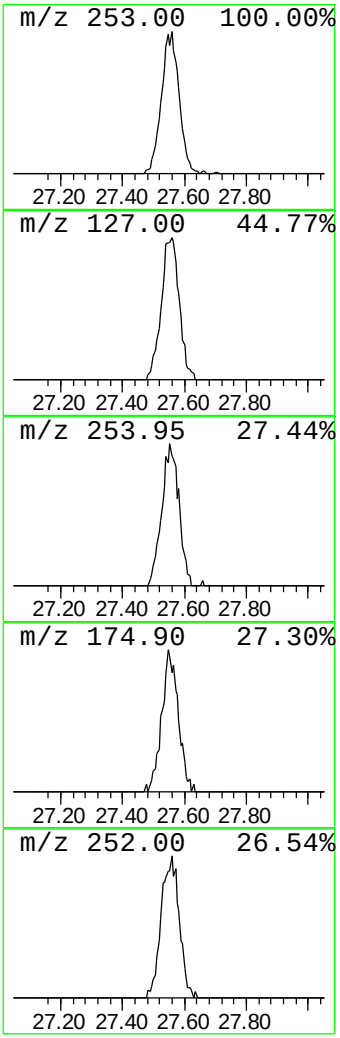
****

Peak Number 10 unknown27.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.55	4.75 ng	101399	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 2-iodo-5-methyl-4-nitro-	253	C4H4IN3O2	149510-86-1	43
2	6-Chloro-2-methyl-4-phenyl-quino...	253	C16H12ClN	022609-12-7	17
3	1,2'-Binaphthalene	254	C20H14	004325-74-0	10
4	1H-Indene, 1,1'-(1,2-ethanediyli...	254	C20H14	072088-04-1	9
5	5-(4-Methoxycinnamoyl)-2-methyl-...	253	C16H15NO2	094298-96-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

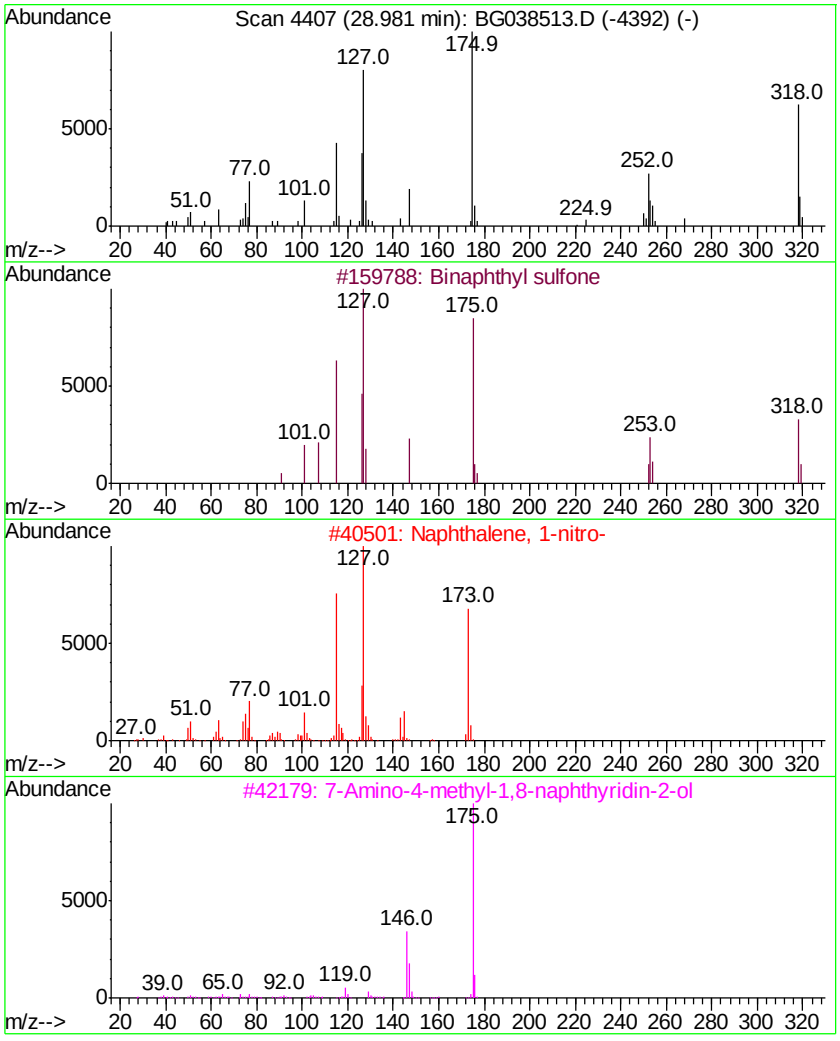
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

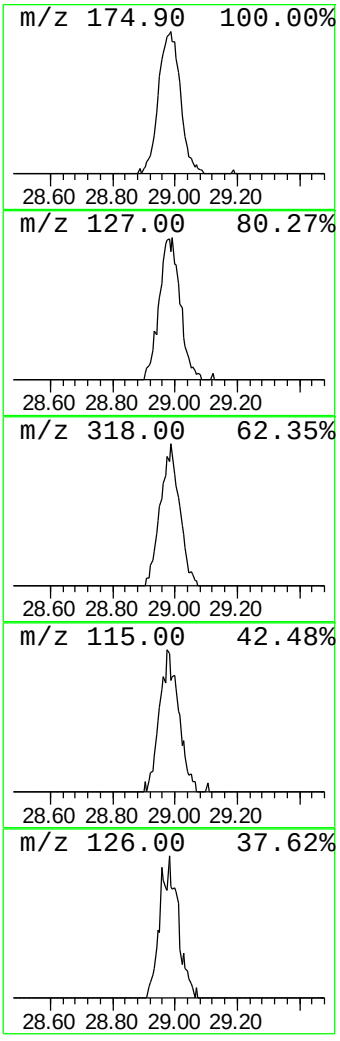
****

Peak Number 11 Binaphthyl sulfone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.98	7.12 ng	151826	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Binaphthyl sulfone	318	C20H14O2S	032390-26-4	52
2	Naphthalene, 1-nitro-	173	C10H7NO2	000086-57-7	16
3	7-Amino-4-methyl-1,8-naphthyridi...	175	C9H9N3O	001569-15-9	14
4	Thiazole, 5-methyl-4-phenyl-	175	C10H9NS	001826-18-2	14
5	2-tert-Butyl-4-methyl-6-(a-methy...	268	C19H24O	001706-65-6	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121218\
Data File : BG038513.D
Acq On : 13 Dec 2018 00:41
Operator : JU/SJ
Sample : J6344-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200031

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	13.3	ng	87436	1	8.06	131553	20.0
3-Penten-2-one, 4...	4.53	25.3	ng	166213	1	8.06	131553	20.0
2-Pentanone, 4-hy...	5.14	37.1	ng	243951	1	8.06	131553	20.0
unknown6.11	6.11	4.0	ng	26531	1	8.06	131553	20.0
unknown7.59	7.59	89.3	ng	587649	1	8.06	131553	20.0
Benzenethiol, 4-(...	14.19	3.0	ng	47732	3	14.70	319864	20.0
unknown14.51	14.51	2.7	ng	42620	3	14.70	319864	20.0
5-Octadecene, (E)-	18.44	20.0	ng	109015	4	17.45	109015	20.0
unknown27.55	27.55	4.8	ng	101399	6	25.01	426529	20.0
Binaphthyl sulfone	28.98	7.1	ng	151826	6	25.01	426529	20.0