LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

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:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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	5.038	368	374	382	rBV2	20951	42060	2.68%	0.399%
2	5.543	453	460	483	rBV	188026	369706	23.57%	3.504%
3	7.182	731	739	751	rBV	149344	313939	20.02%	2.975%
4	7.523	790	797	809	rBV	313746	617029	39.34%	5.848%
5	7.987	870	876	887	rVB	60331	113005	7.20%	1.071%
6	8.310	920	931	943	rBV	254771	489734	31.22%	4.641%
7	9.162	1069	1076	1090	rBV	183702	391593	24.97%	3.711%
8	9.909	1194	1203	1208	rBV	503065	877613	55.95%	8.317%
9	9.973	1208	1214	1231	rVB	581701	1041204	66.38%	9.868%
10	10.191	1244	1251	1264	rBV	342586	634048	40.42%	6.009%
11	10.807	1349	1356	1365	rVB	106400	209594	13.36%	1.986%
12	11.248	1420	1431	1438	rBV10	6234	23839	1.52%	0.226%
13	12.235	1591	1599	1608	rBV2	37921	84202	5.37%	0.798%
14	12.500	1639	1644	1652	rVB9	10137	20648	1.32%	0.196%
15	12.646	1662	1669	1676	rBV	58954	103208	6.58%	0.978%
16	12.764	1682	1689	1697	rVB8	9678	25720	1.64%	0.244%
17	13.252	1764	1772	1784	rBV	726126	1255920	80.07%	11.903%
18	13.399	1791	1797	1803	rBV	17480	34753	2.22%	0.329%
19	14.632	2001	2007	2017	rBV2	192048	352720	22.49%	3.343%
20	16.131	2255	2262	2276	rVB	475122	825930	52.66%	7.828%
21	16.577	2334	2338	2343	rVB3	29540	44546	2.84%	0.422%
22	16.842	2379	2383	2389	rBV	10883	22595	1.44%	0.214%
23	17.382	2469	2475	2482	rBV2	228974	374432	23.87%	3.549%
24	19.809	2884	2888	2894	rVB	36305	53402	3.40%	0.506%
25	19.979	2911	2917	2924	rBV	1099345	1568498	100.00%	14.865%
26	21.642	3194	3200	3208	rBV2	186533	346513	22.09%	3.284%
27	24.844	3736	3745	3756	rVB2	104394	315003	20.08%	2.985%

Sum of corrected areas: 10551454

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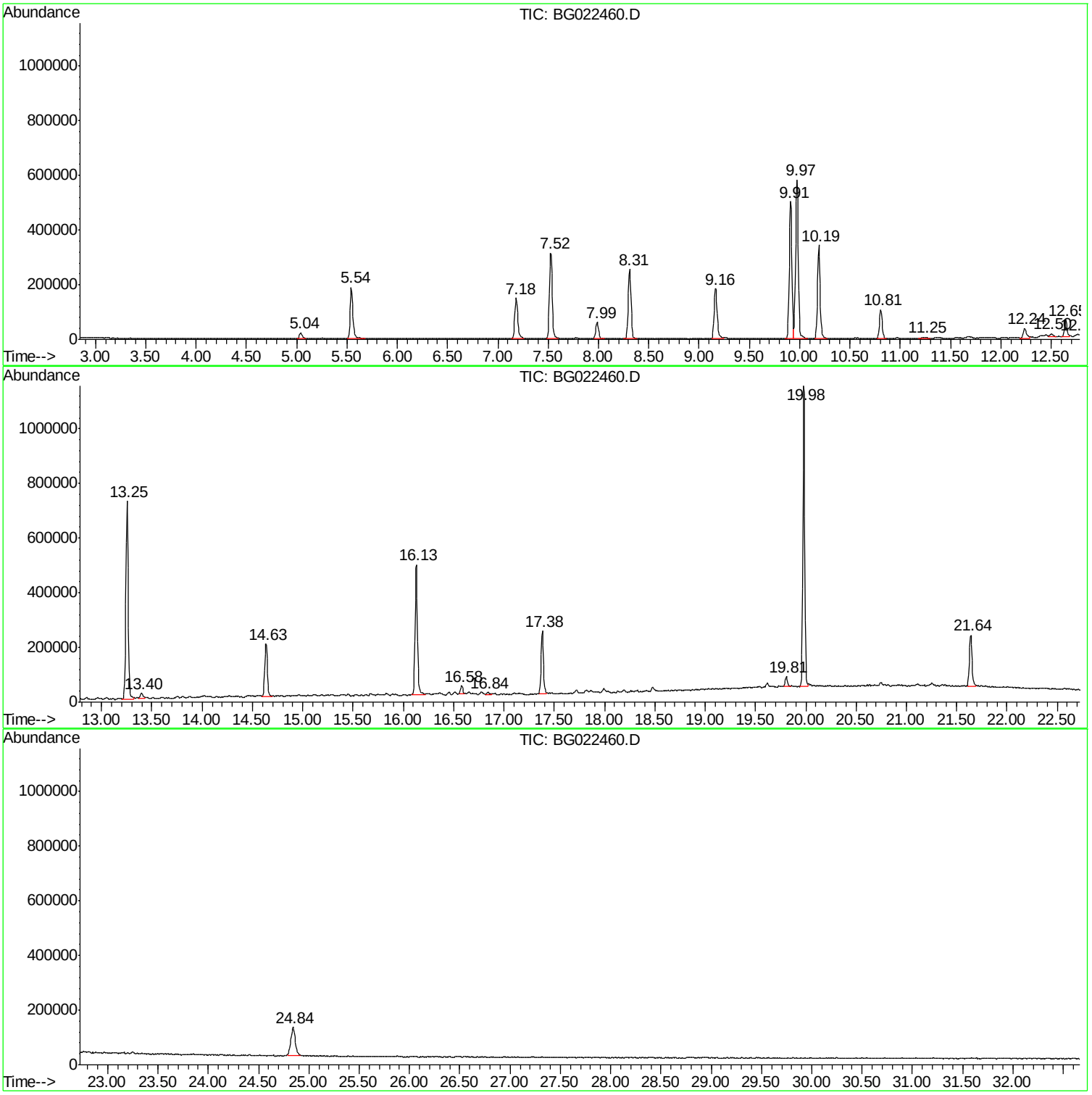
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
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TIC Library : C:\DATABASE\NIST02.L
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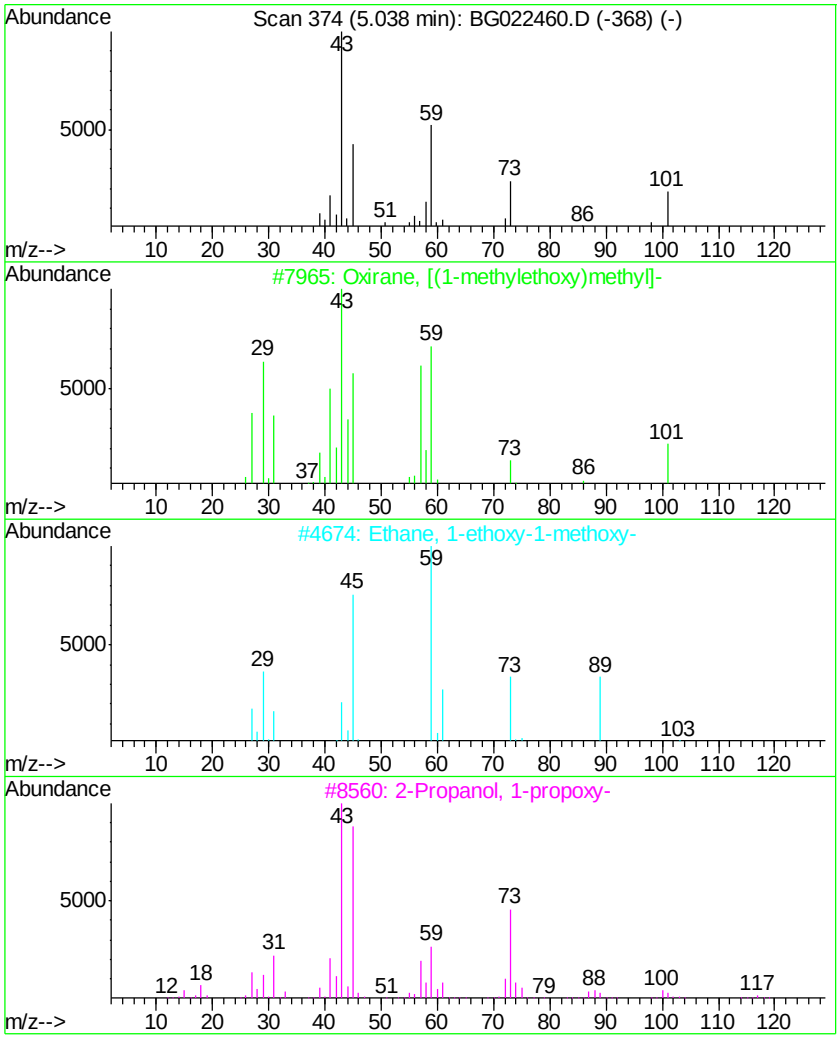
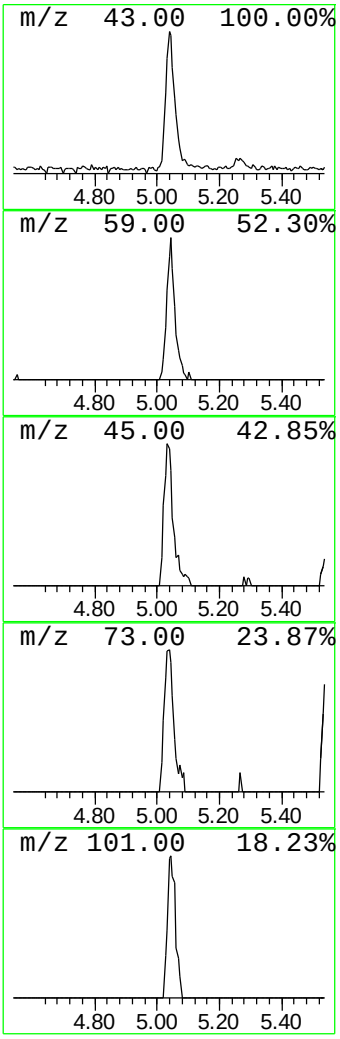
****

Peak Number 1 unknown5.04 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	7.44 ng	42060	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	45
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	33
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	28
4	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	25





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Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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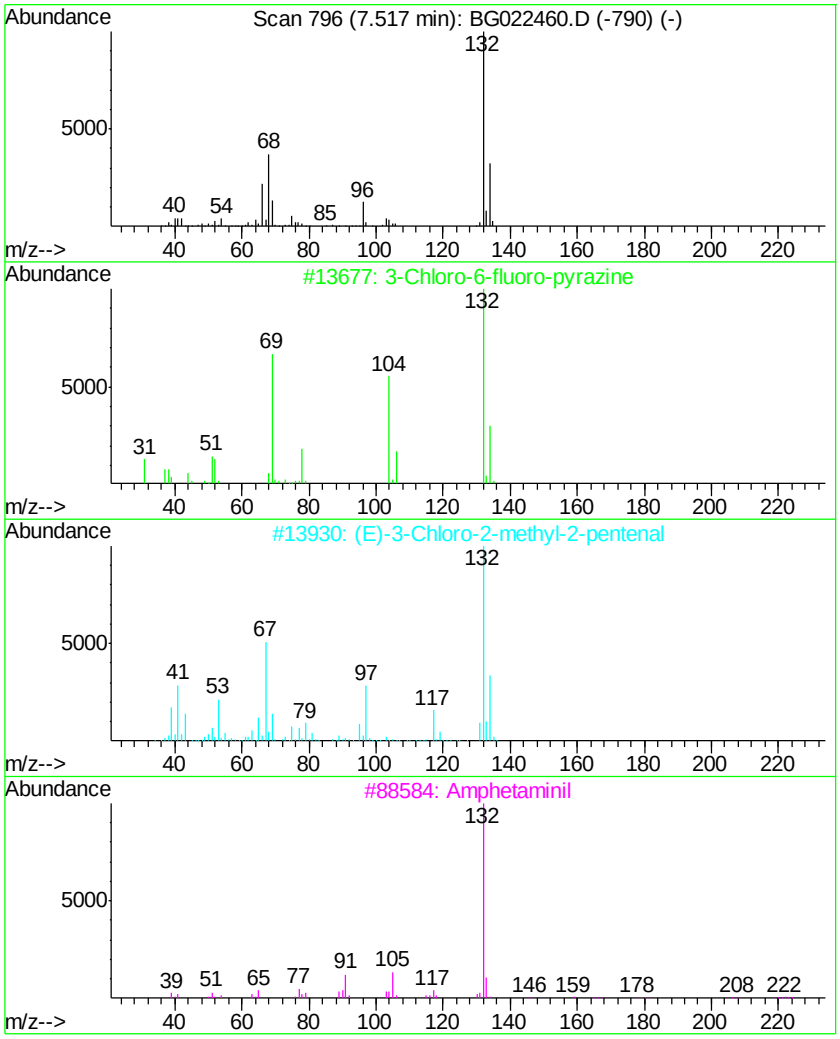
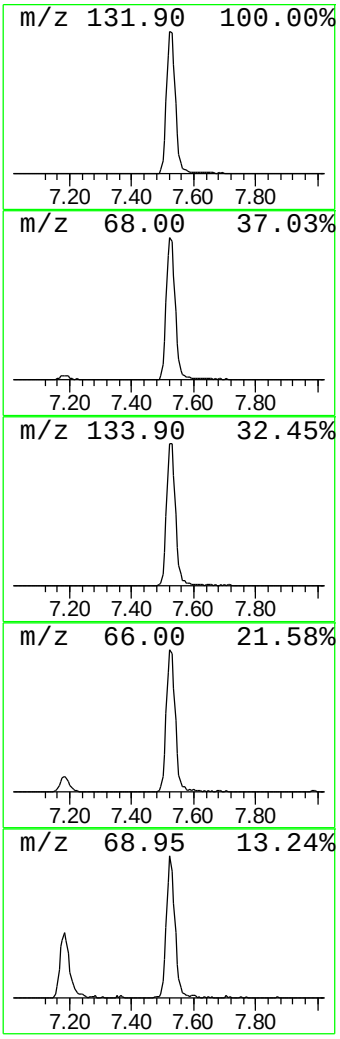
Peak Number 2 unknown7.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	109.20 ng	617029	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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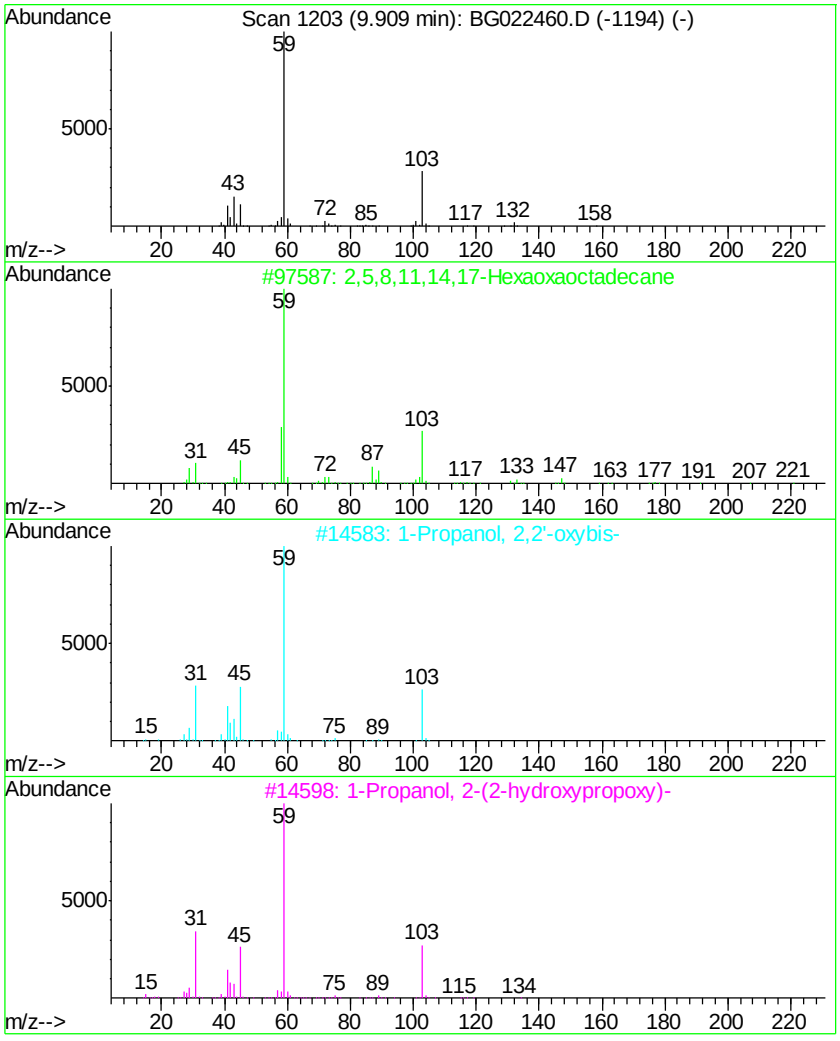
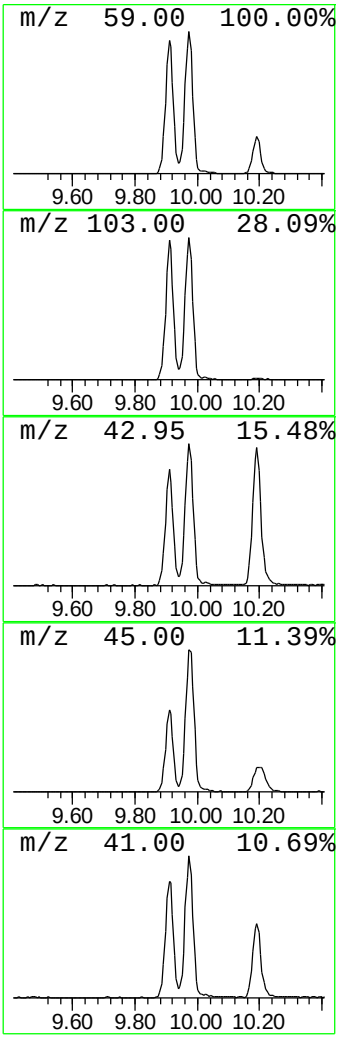
Peak Number 4 2,5,8,11,14,17-Hexaoxaoctad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.91	83.74 ng	877613	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	74
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
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Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

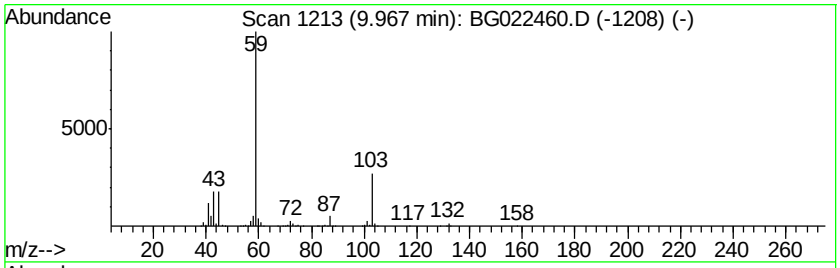
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

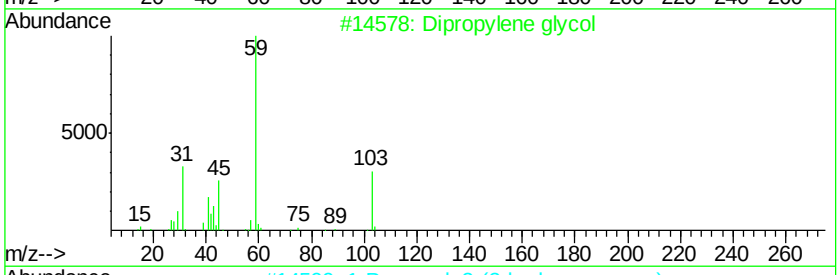
****

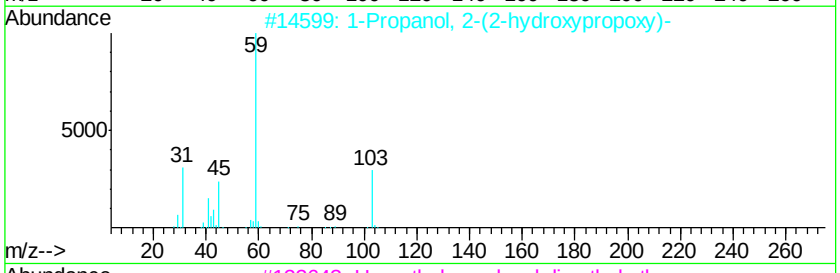
Peak Number 5 Dipropylene glycol Concentration Rank 2

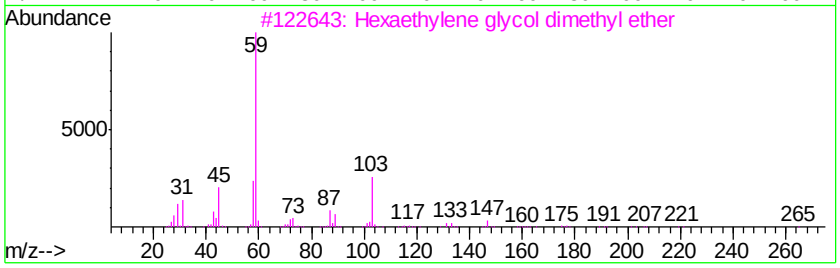
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	99.35 ng	1041200	Naphthalene-d8	10.81

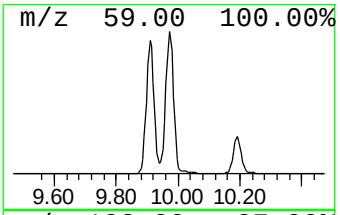
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dipropylene glycol	134	C6H14O3	025265-71-8	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	74
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	72
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64

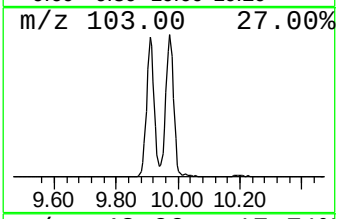


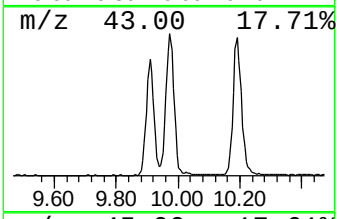


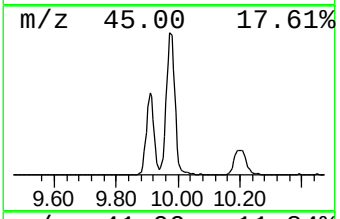


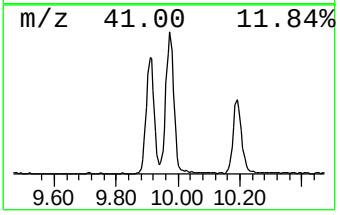












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Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

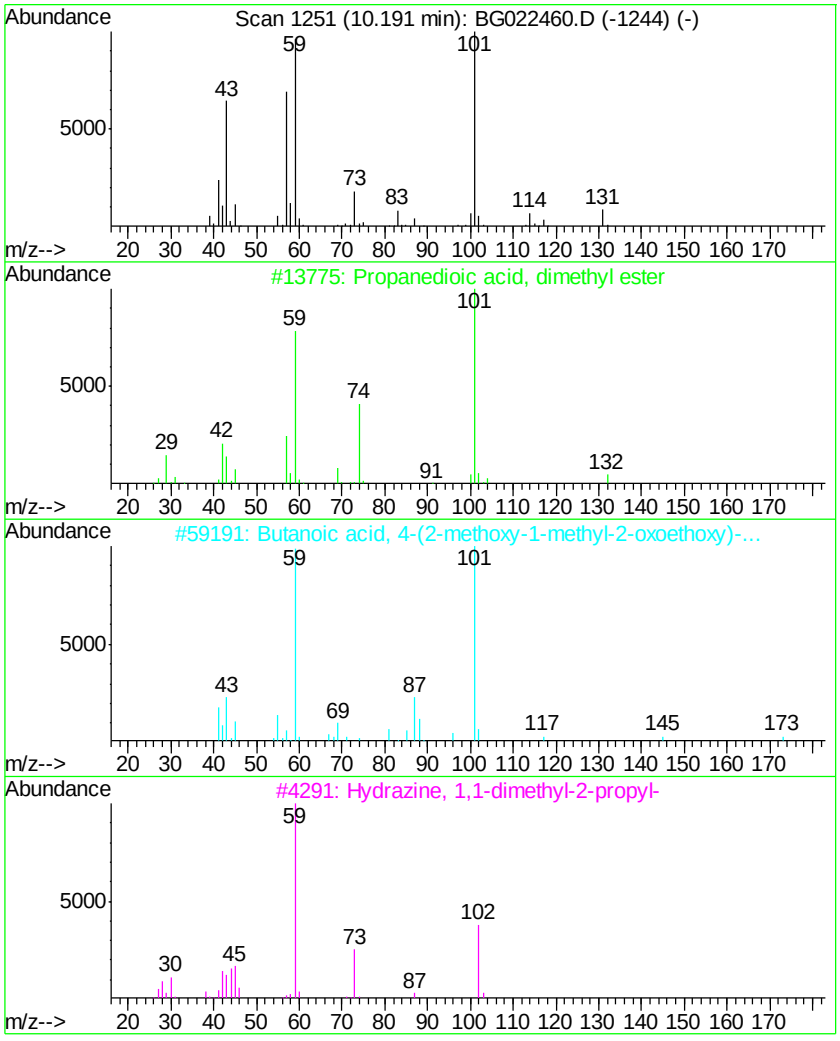
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

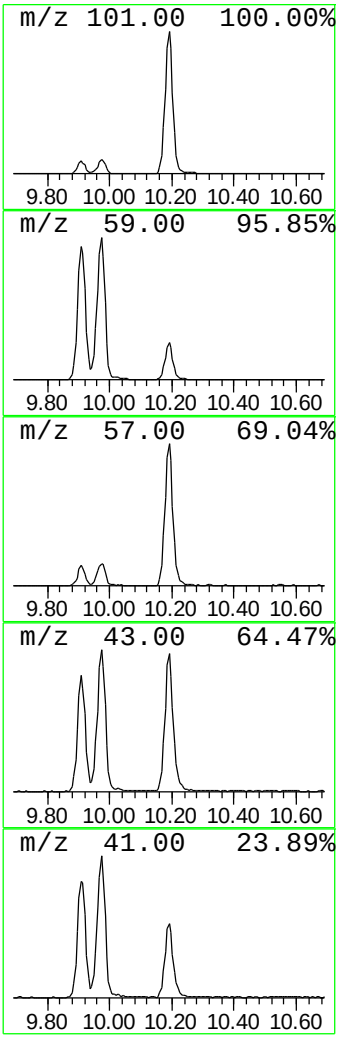
****

Peak Number 6 Propanedioic acid, dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	60.50 ng	634048	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	56
2	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	50
3	Hydrazine, 1,1-dimethyl-2-propyl-	102	C5H14N2	052728-54-8	35
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	32
5	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	27





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TIC Library : C:\DATABASE\NIST02.L
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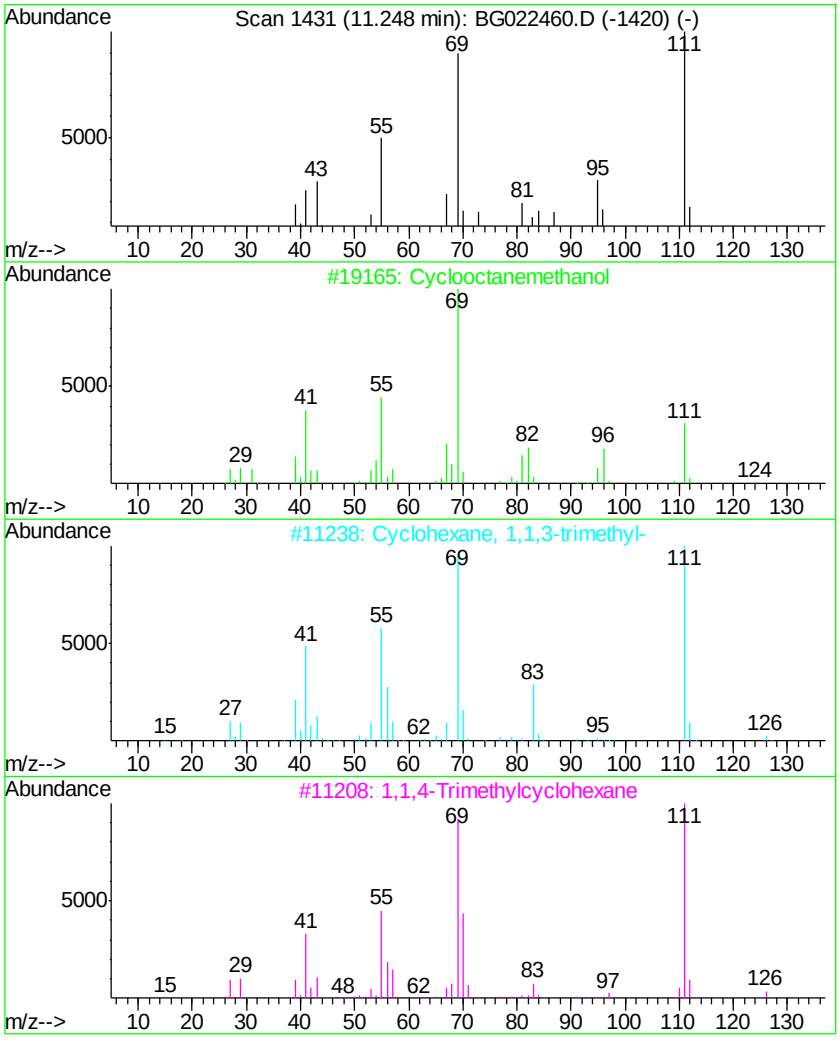
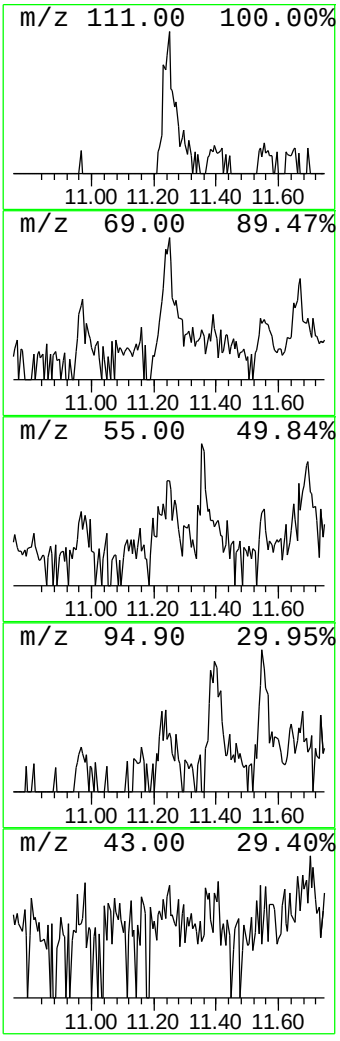
****

Peak Number 7 Cyclooctanemethanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.27 ng	23839	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctanemethanol	142	C9H18O	003637-63-6	59
2	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	53
3	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	36
4	4-Methyl-2-heptene	112	C8H16	003404-56-6	35
5	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	35





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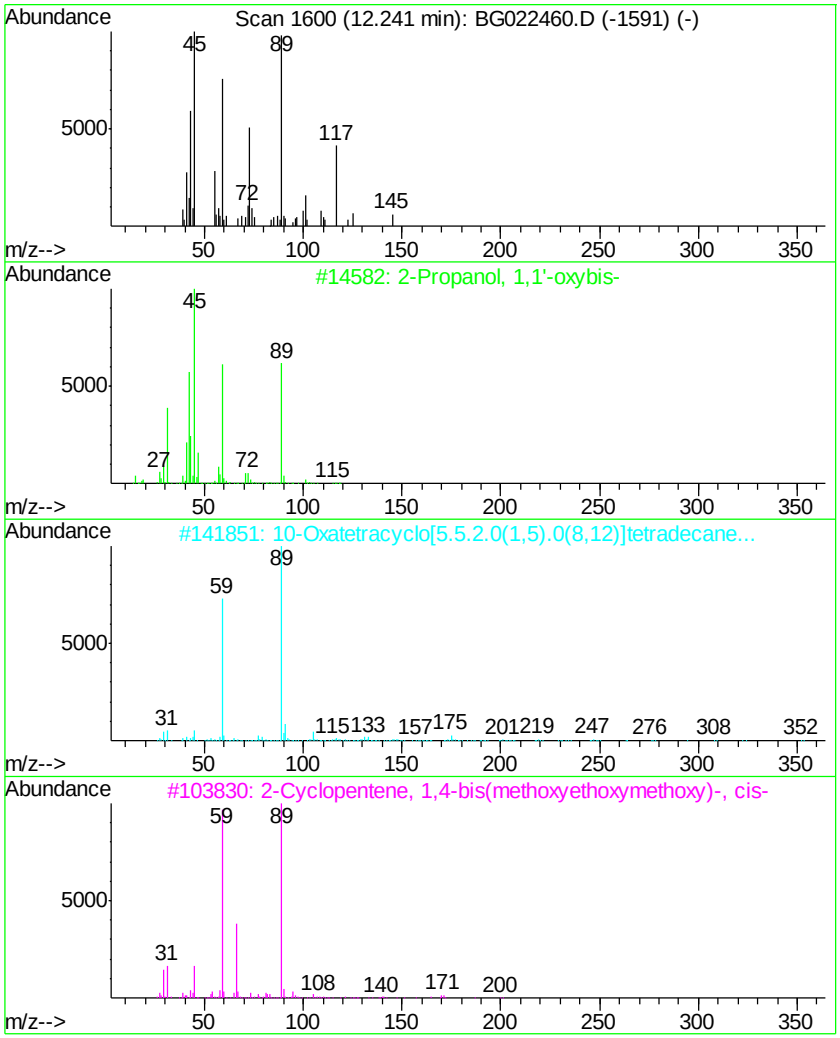
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

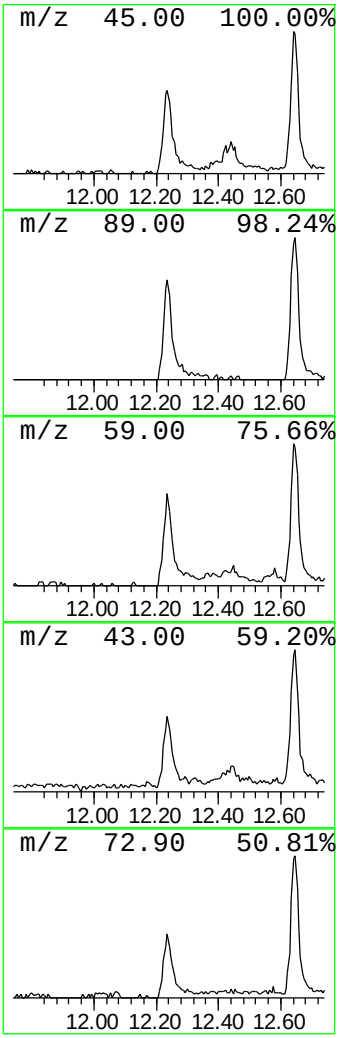
****

Peak Number 8 2-Propanol, 1,1'-oxybis- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	8.03 ng	84202	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	64
2	10-Oxatetracyclo[5.5.2.0(1,5).0(...	352	C18H24O7	1000154-01-5	45
3	2-Cyclopentene, 1,4-bis(methoxye...	276	C13H24O6	1000156-00-3	38
4	Propane, 1,2,3-trimethoxy-	134	C6H14O3	020637-49-4	38
5	Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
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Instrument : BNA_G
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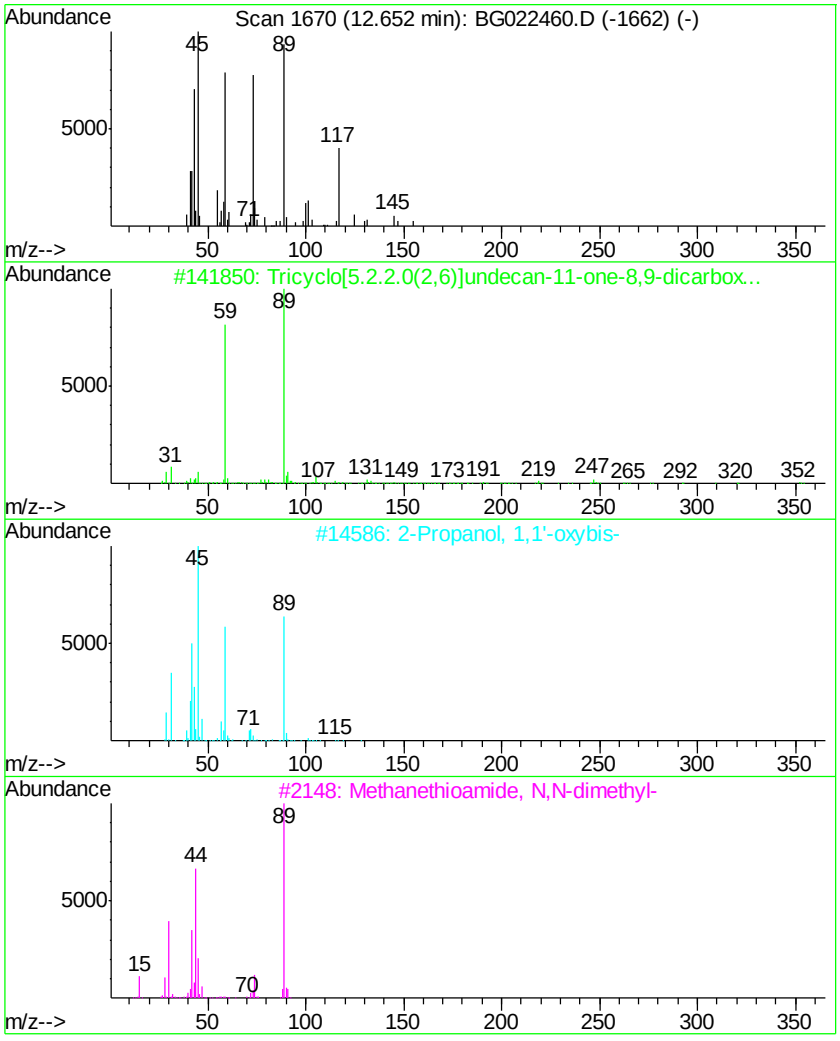
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

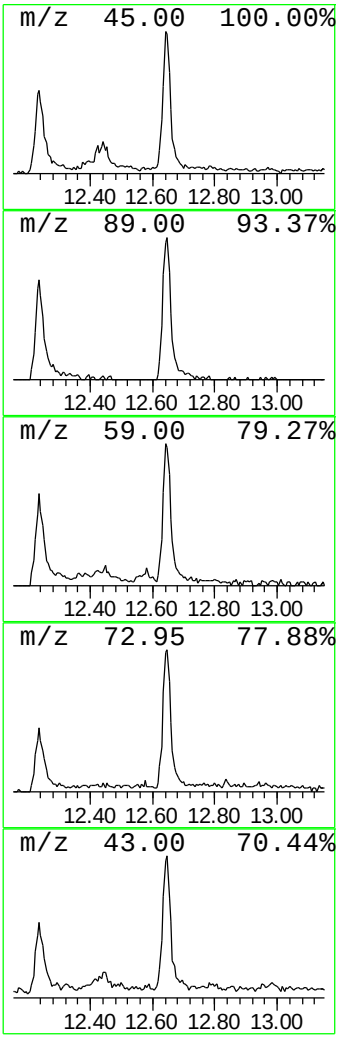
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Tricyclo[5.2.2.0(2,6)]undec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	9.85 ng	103208	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	53
2	2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	50
3	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	50
4	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	50
5	N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	47





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

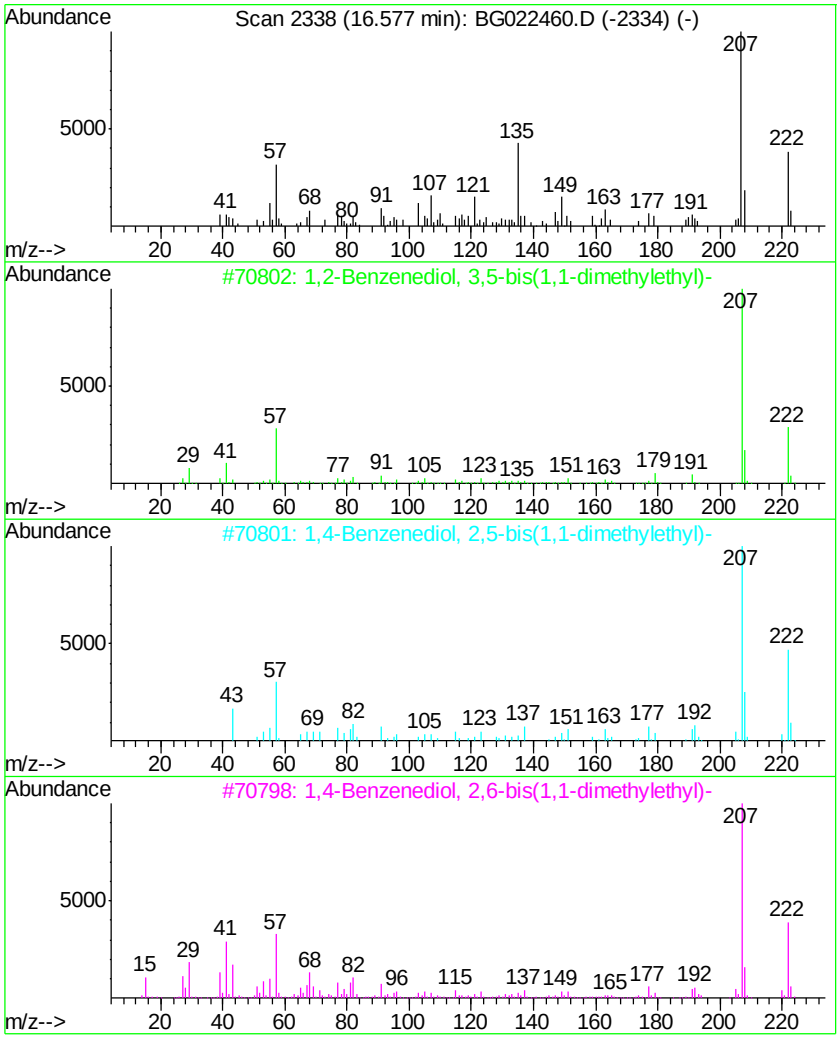
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

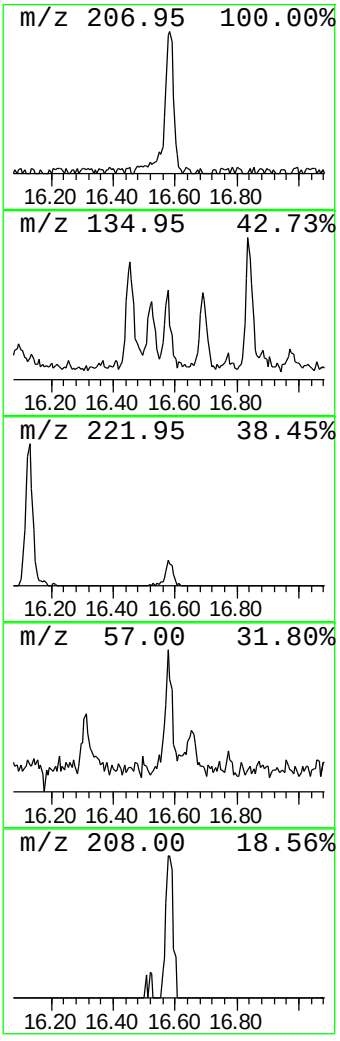
****

Peak Number 10 1,2-Benzenediol, 3,5-bis(1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	2.38 ng	44546	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 3,5-bis(1,1-dim...	222	C14H22O2	001020-31-1	64
2	1,4-Benzenediol, 2,5-bis(1,1-dim...	222	C14H22O2	000088-58-4	60
3	1,4-Benzenediol, 2,6-bis(1,1-dim...	222	C14H22O2	002444-28-2	53
4	2,4-Di-tert-butylthiophenol	222	C14H22S	019728-43-9	52
5	5H-Benzo[b]pyran-8-ol, 2,3,5,5,8...	222	C14H22O2	097306-66-6	49





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

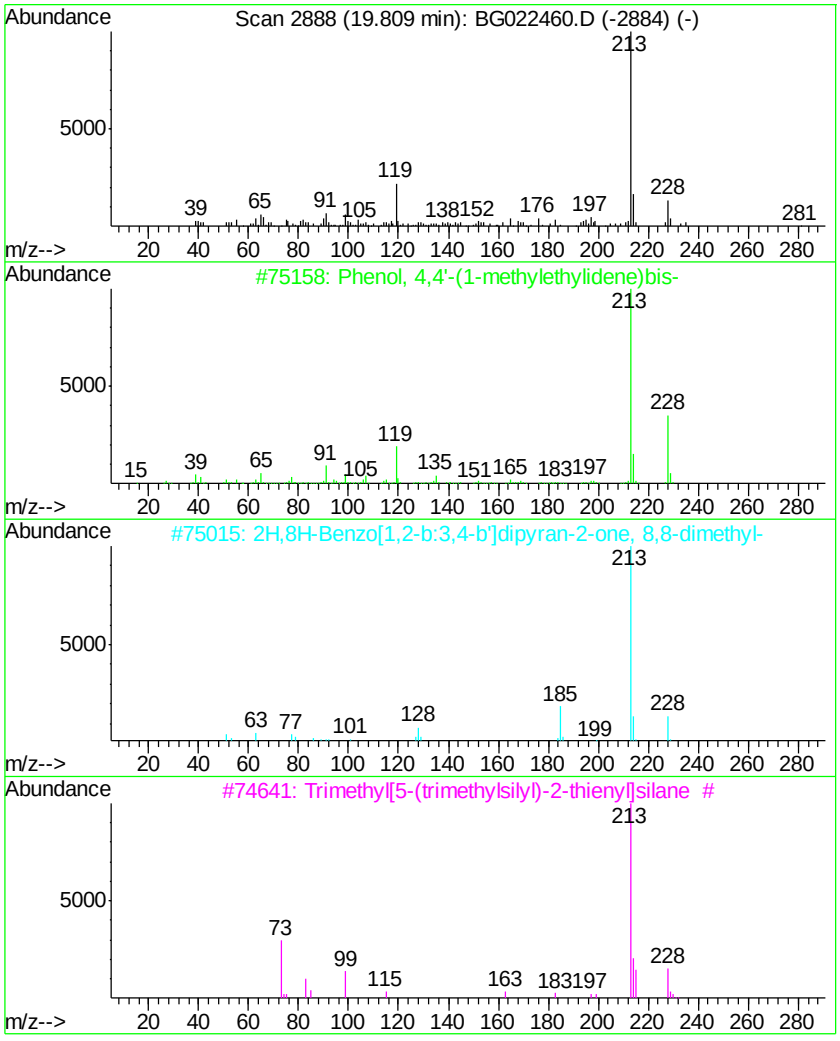
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

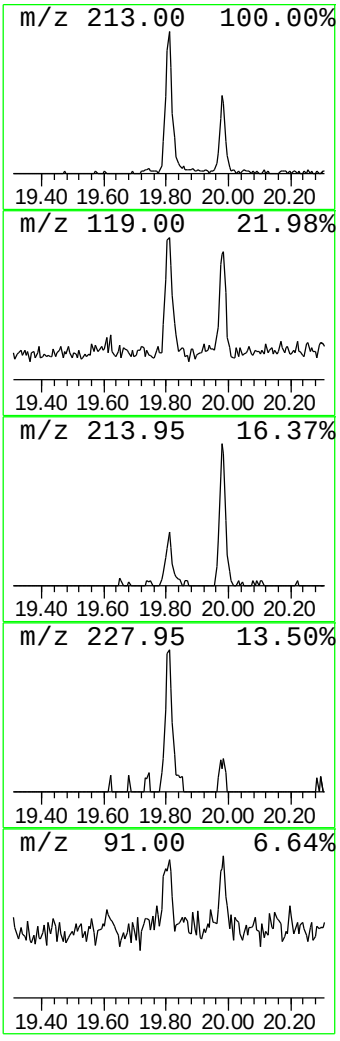
****

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.81	3.08 ng	53402	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
3	Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	59
4	Imidazole, 5-trifluoromethyl-2-(...	213	C9H6F3N3	033468-83-6	50
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062016\
Data File : BG022460.D
Acq On : 21 Jun 2016 3:41
Operator : UM/SJ
Sample : H3679-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-28

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.04	5.04	7.4	ng	42060	1	7.99	113005	20.0
unknown7.52	7.52	109.2	ng	617029	1	7.99	113005	20.0
2,5,8,11,14,17-He...	9.91	83.7	ng	877613	2	10.81	209594	20.0
Dipropylene glycol	9.97	99.3	ng	1041200	2	10.81	209594	20.0
Propanedioic acid...	10.19	60.5	ng	634048	2	10.81	209594	20.0
Cyclooctanemethanol	11.25	2.3	ng	23839	2	10.81	209594	20.0
2-Propanol, 1,1'-...	12.24	8.0	ng	84202	2	10.81	209594	20.0
Tricyclo[5.2.2.0(...	12.65	9.8	ng	103208	2	10.81	209594	20.0
1,2-Benzenediol, ...	16.58	2.4	ng	44546	4	17.38	374432	20.0
Phenol, 4,4'-(1-m...	19.81	3.1	ng	53402	5	21.64	346513	20.0