LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

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_F\METHODS\8270-BF092415.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	2.217	6	7	31	rVB2	68141	247123	6.20%	0.854%
2	5.143	260	263	265	rVB	342549	438589	11.00%	1.517%
3	5.543	295	298	300	rBV	1609027	1397060	35.03%	4.831%
4	6.560	385	387	390	rBV	661158	771930	19.36%	2.669%
5	6.720	398	401	403	rBV	2644741	2964010	74.33%	10.249%
6	6.880	412	415	416	rBV	85975	97486	2.44%	0.337%
7	6.949	419	421	424	rBV	895855	815753	20.46%	2.821%
8	7.109	432	435	437	rBV	3272908	2787160	69.89%	9.637%
9	7.520	468	471	473	rVB	2512058	2464115	61.79%	8.520%
10	8.240	531	534	536	rBV	1209651	1050444	26.34%	3.632%
11	8.458	551	553	554	rBV	47965	82859	2.08%	0.287%
12	8.480	554	555	557	rVV	103278	80495	2.02%	0.278%
13	8.560	561	562	568	rVV2	31008	48711	1.22%	0.168%
14	8.743	573	578	584	rVV2	89684	255884	6.42%	0.885%
15	8.835	584	586	590	rVV2	332315	599726	15.04%	2.074%
16	8.949	594	596	598	rVB	251569	212270	5.32%	0.734%
17	9.315	625	628	630	rBV	4516479	3987883	100.00%	13.789%
18	9.406	635	636	641	rVB	96364	84525	2.12%	0.292%
19	9.703	660	662	664	rBV	268492	214394	5.38%	0.741%
20	9.989	685	687	690	rBV2	1056569	1086398	27.24%	3.756%
21	10.412	723	724	726	rVB	63491	58151	1.46%	0.201%
22	10.629	741	743	747	rBV3	30346	72757	1.82%	0.252%
23	10.778	753	756	759	rBV2	2108211	2445008	61.31%	8.454%
24	10.881	763	765	770	rVB2	56364	108712	2.73%	0.376%
25	11.338	803	805	806	rBV	62606	58876	1.48%	0.204%
26	11.475	815	817	820	rBV	1133703	1028480	25.79%	3.556%
27	12.001	860	863	865	rBV	117906	158156	3.97%	0.547%
28	12.778	929	931	935	rBV	44506	80008	2.01%	0.277%
29	13.064	953	956	959	rBV	3521959	3224697	80.86%	11.150%
30	13.624	1003	1005	1010	rVB	45220	62938	1.58%	0.218%
31	13.955	1031	1034	1036	rBV	56671	85111	2.13%	0.294%
32	14.115	1045	1048	1050	rBV	1031230	961979	24.12%	3.326%
33	15.578	1173	1176	1179	rBV	592296	889064	22.29%	3.074%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-9-15-15

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_F\METHODS\8270-BF092415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 28920752

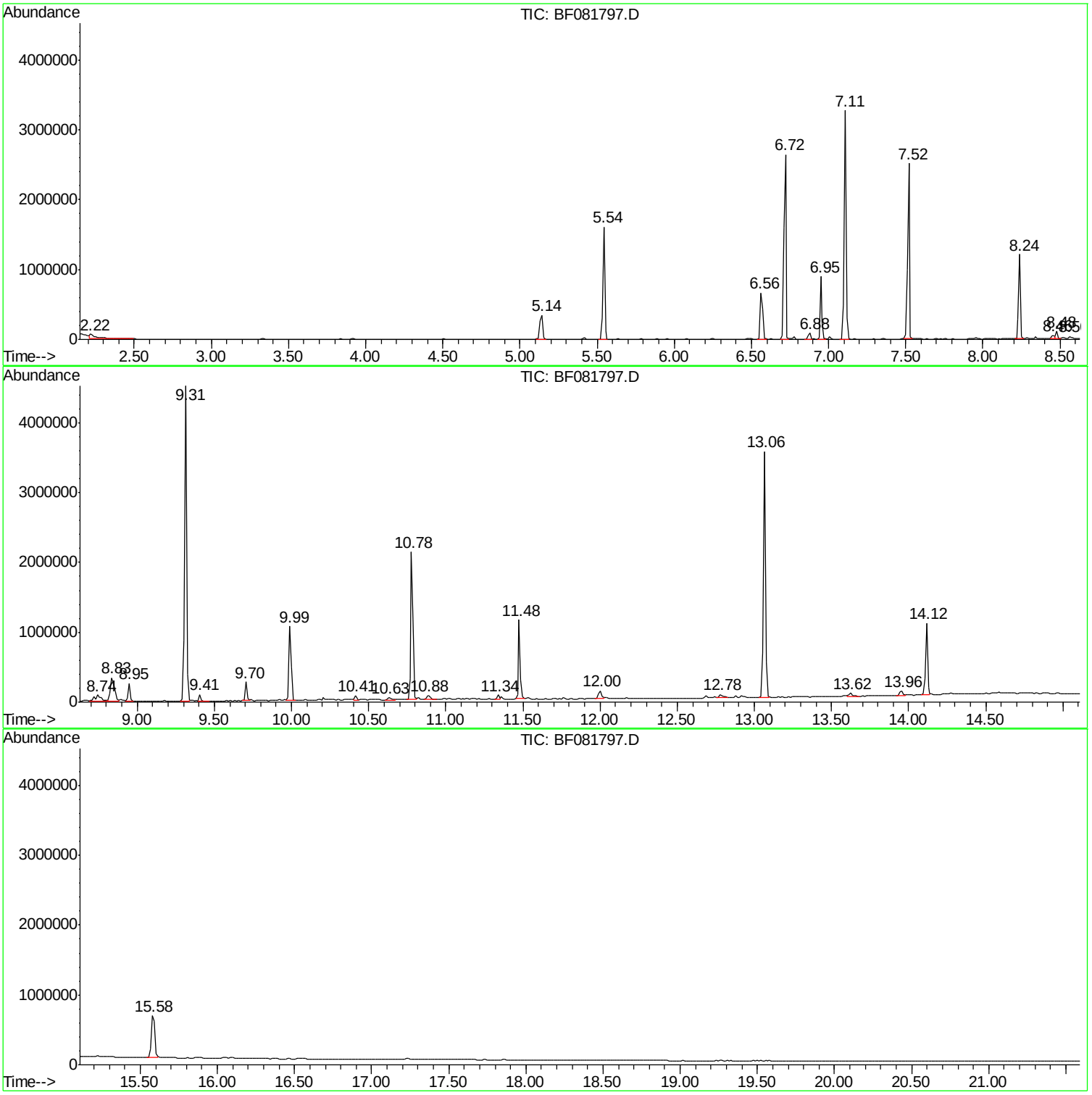
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

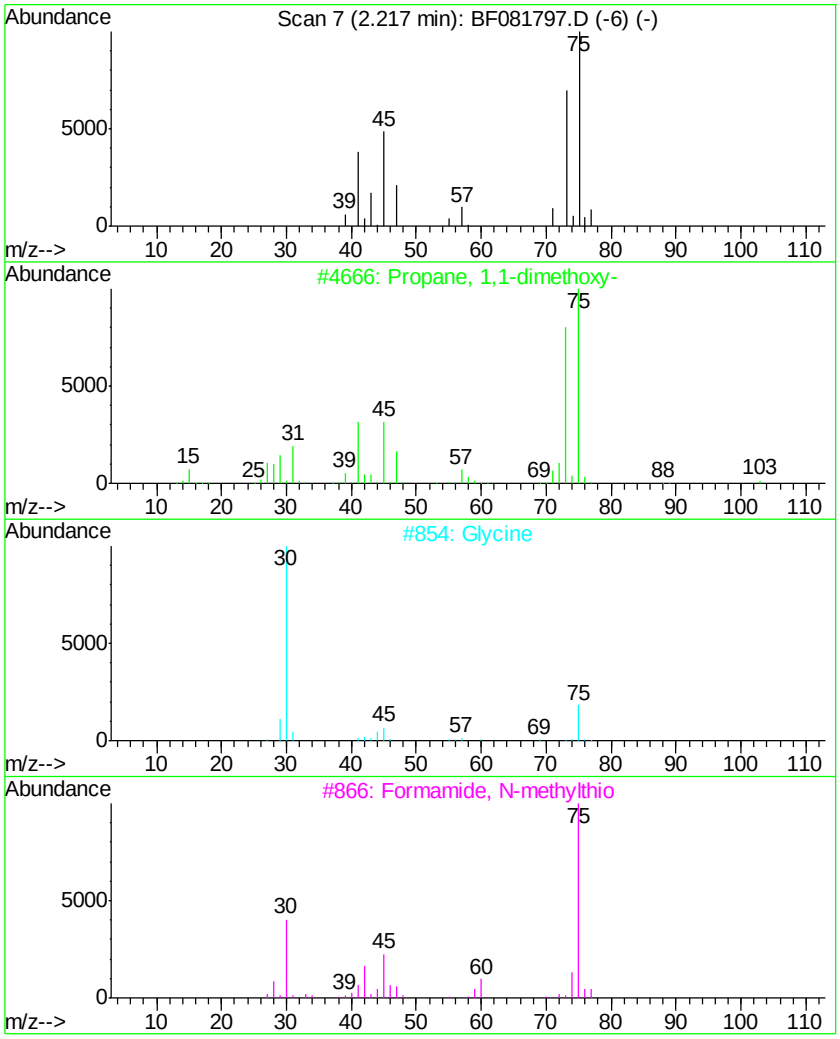
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

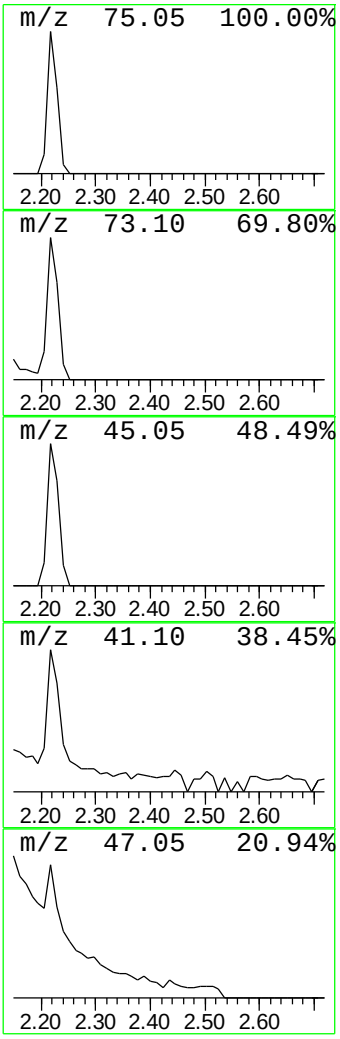
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	6.06 ng	247123	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycine	75	C2H5NO2	000056-40-6	7
3	Formamide, N-methylthio	75	C2H5NS	018952-41-5	5
4	Ethanethioamide	75	C2H5NS	000062-55-5	5
5	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	4





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

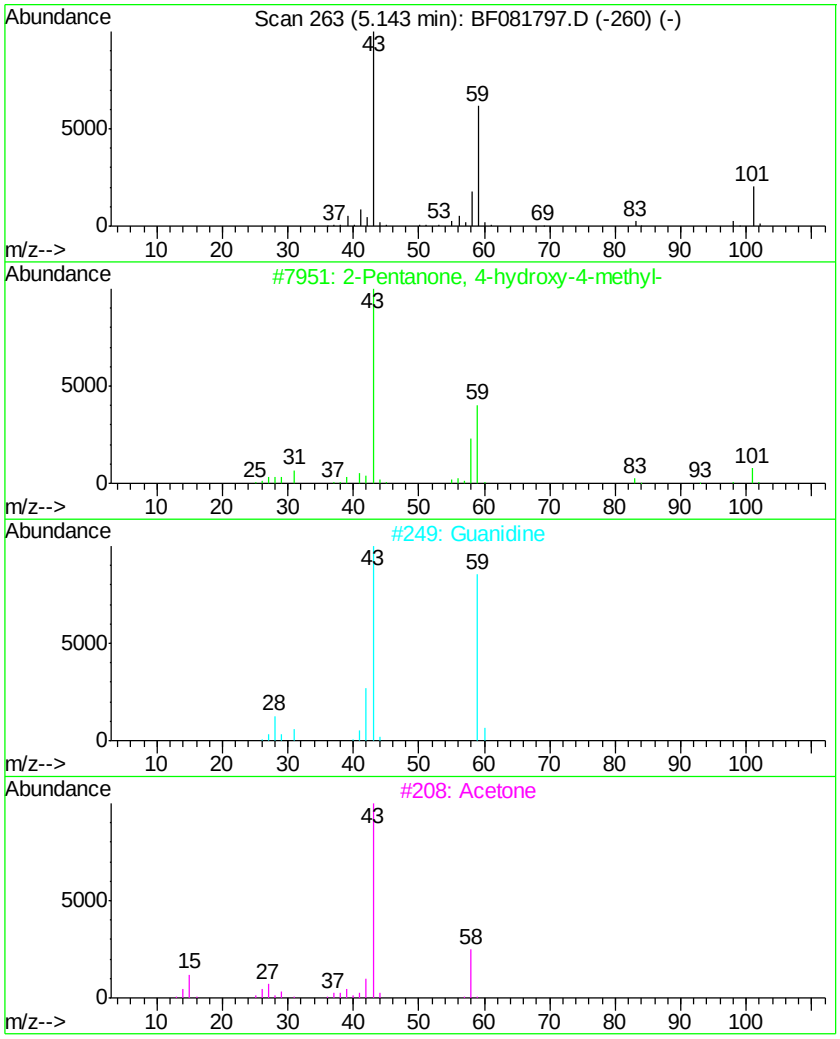
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

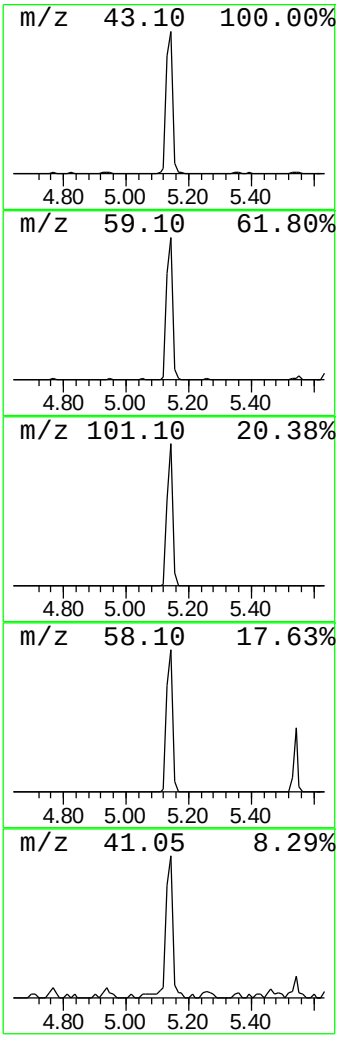
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	10.75 ng	438589	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

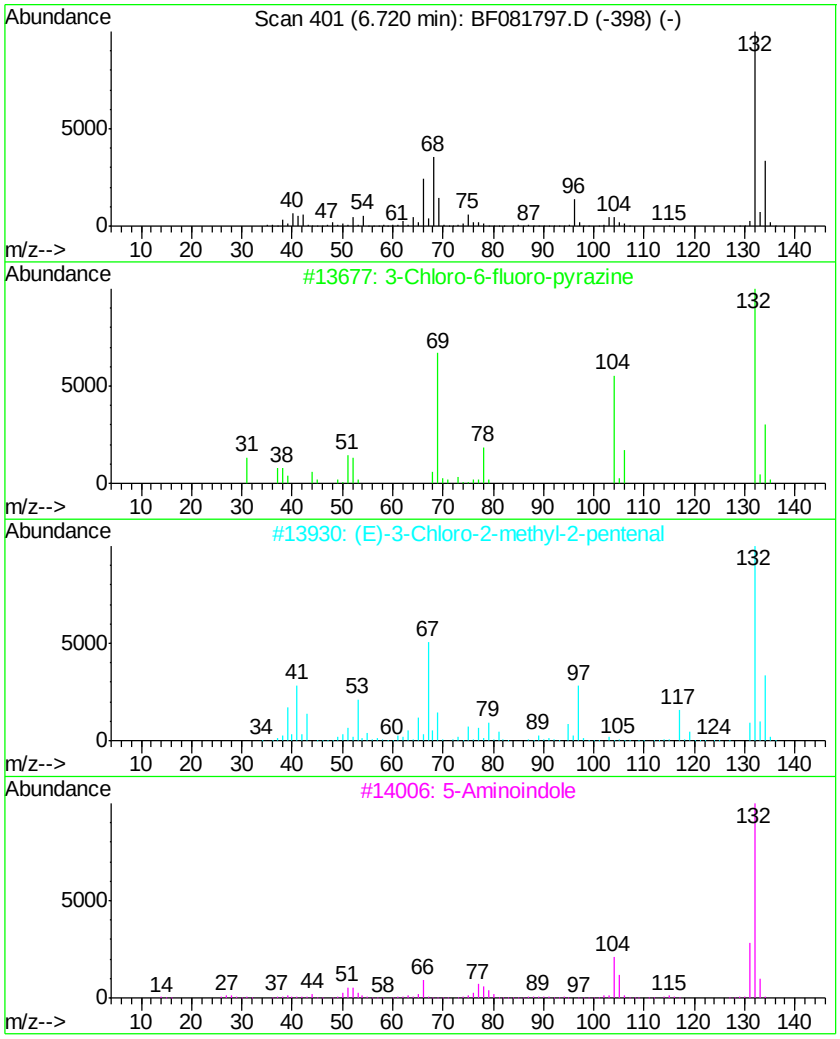
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

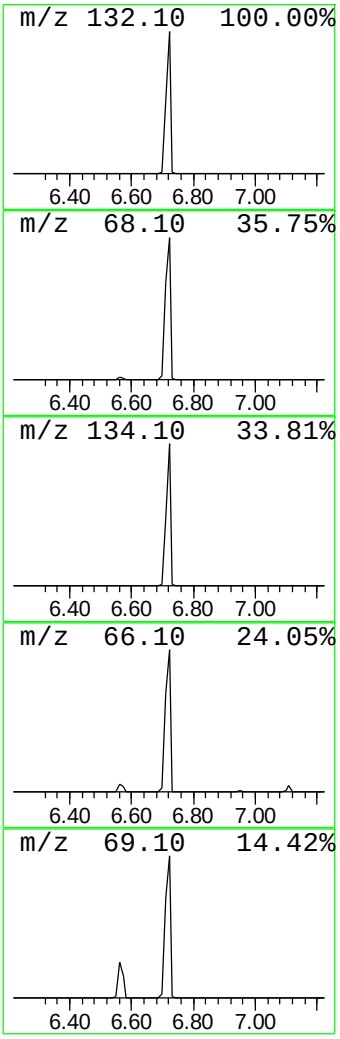
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	72.67 ng	2964010	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

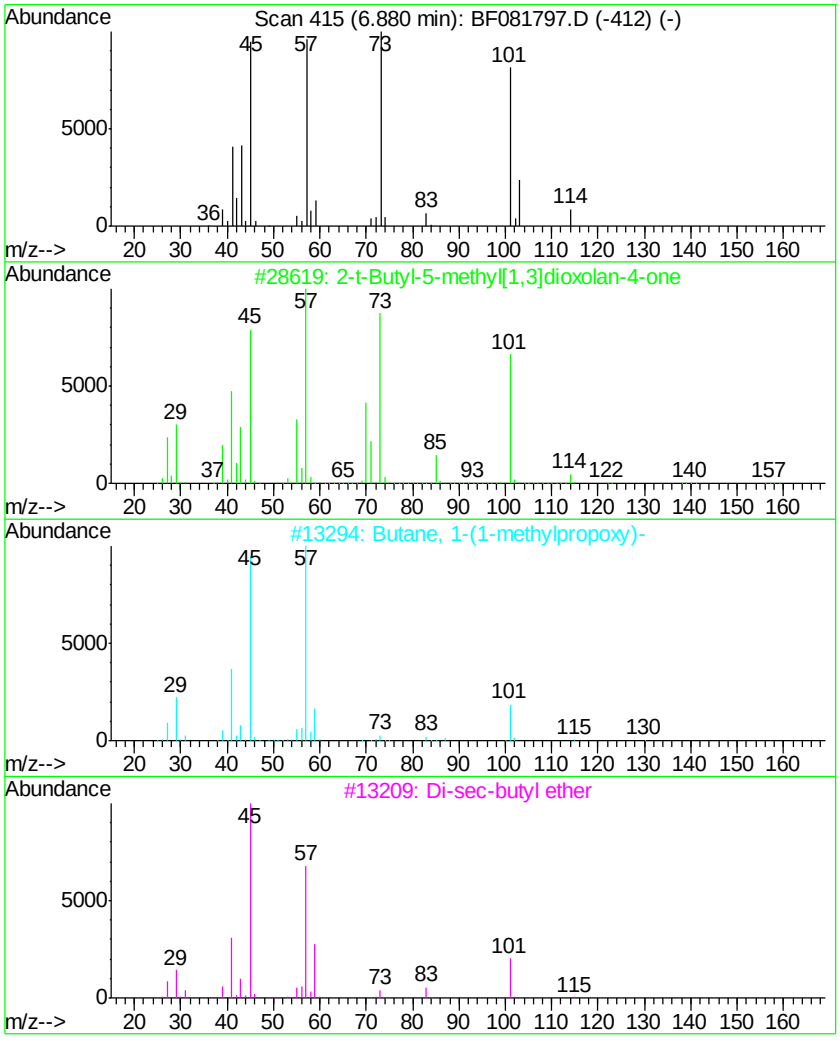
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

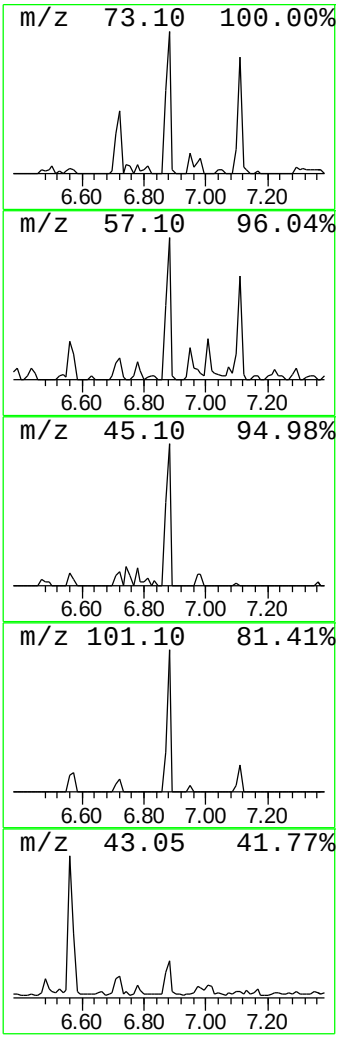
****

Peak Number 4 2-t-Butyl-5-methyl[1,3]diox... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	2.39 ng	97486	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	72
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
4	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	42
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

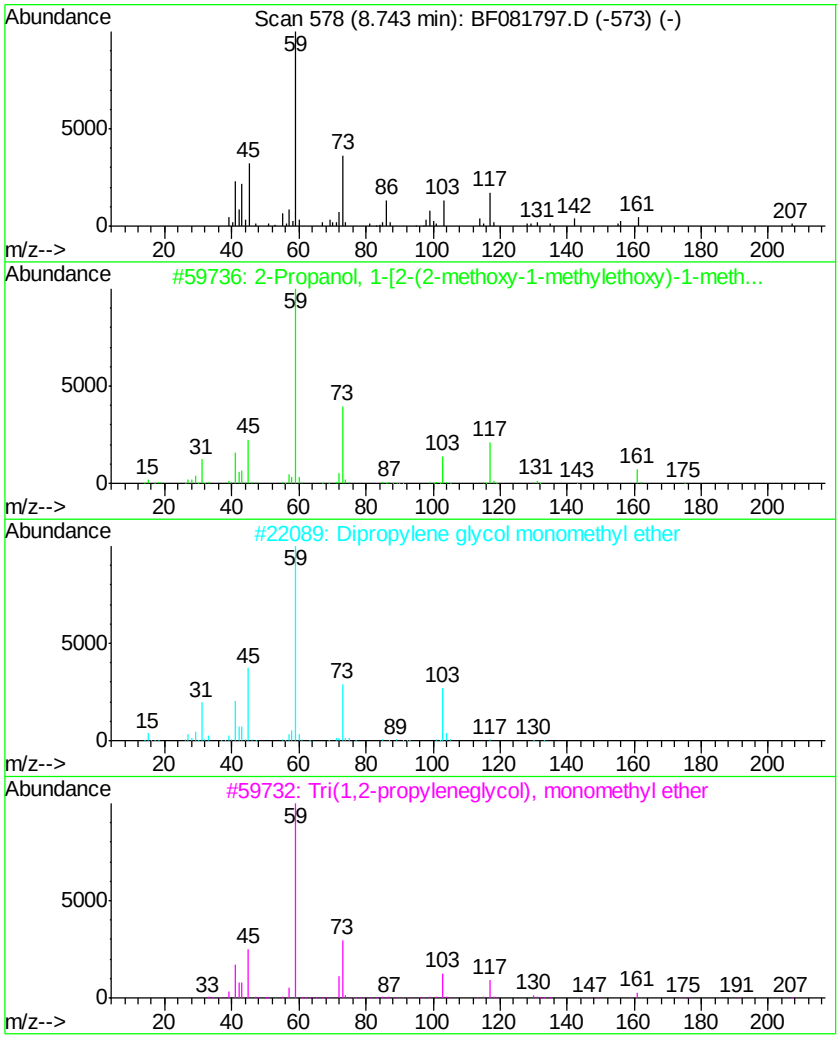
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

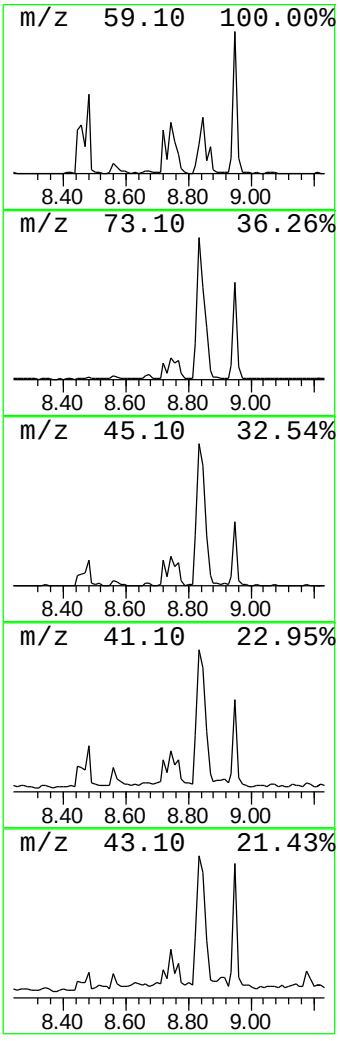
****

Peak Number 6 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.74	4.87 ng	255884	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	72
2	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	59
3	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	56
4	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	47
5	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	45





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

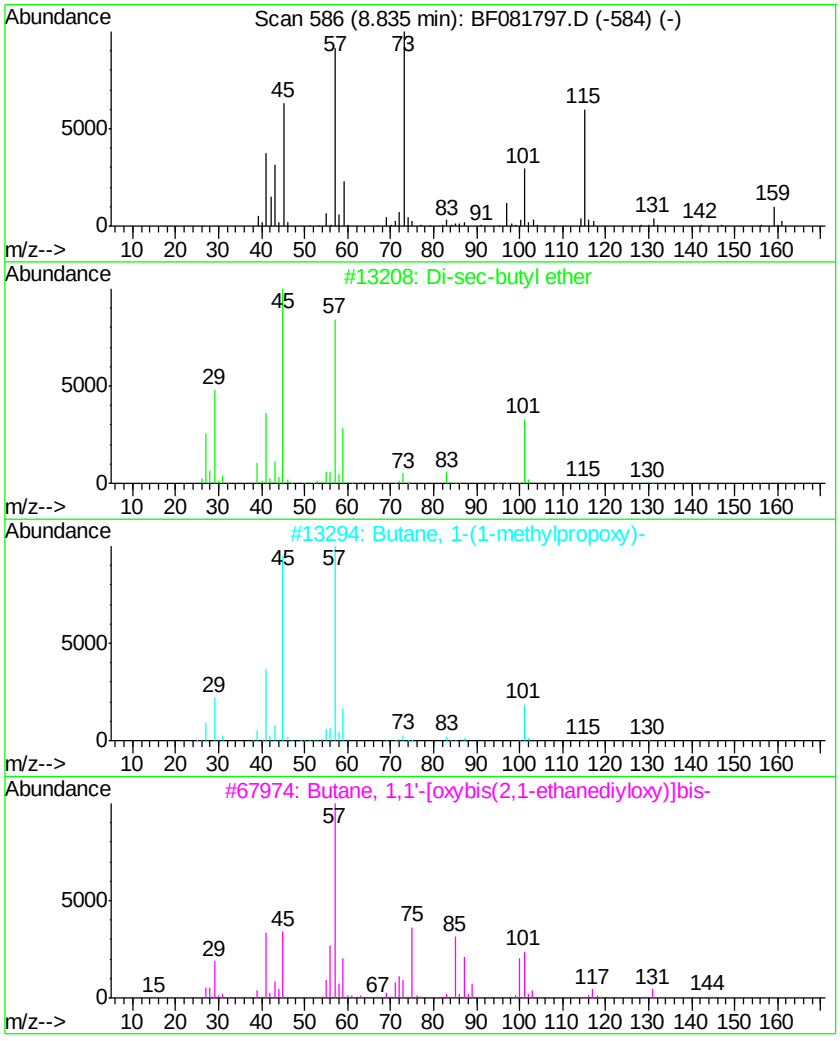
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

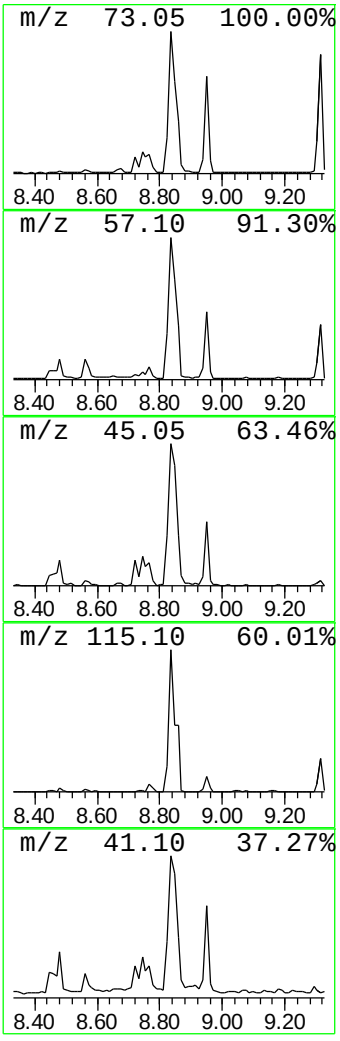
****

Peak Number 7 unknown8.33 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	11.42 ng	599726	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-butyl ether	130	C8H18O	006863-58-7	43
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	35
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	32
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	27
5	(tert-Butoxymethyl)oxirane	130	C7H14O2	007665-72-7	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

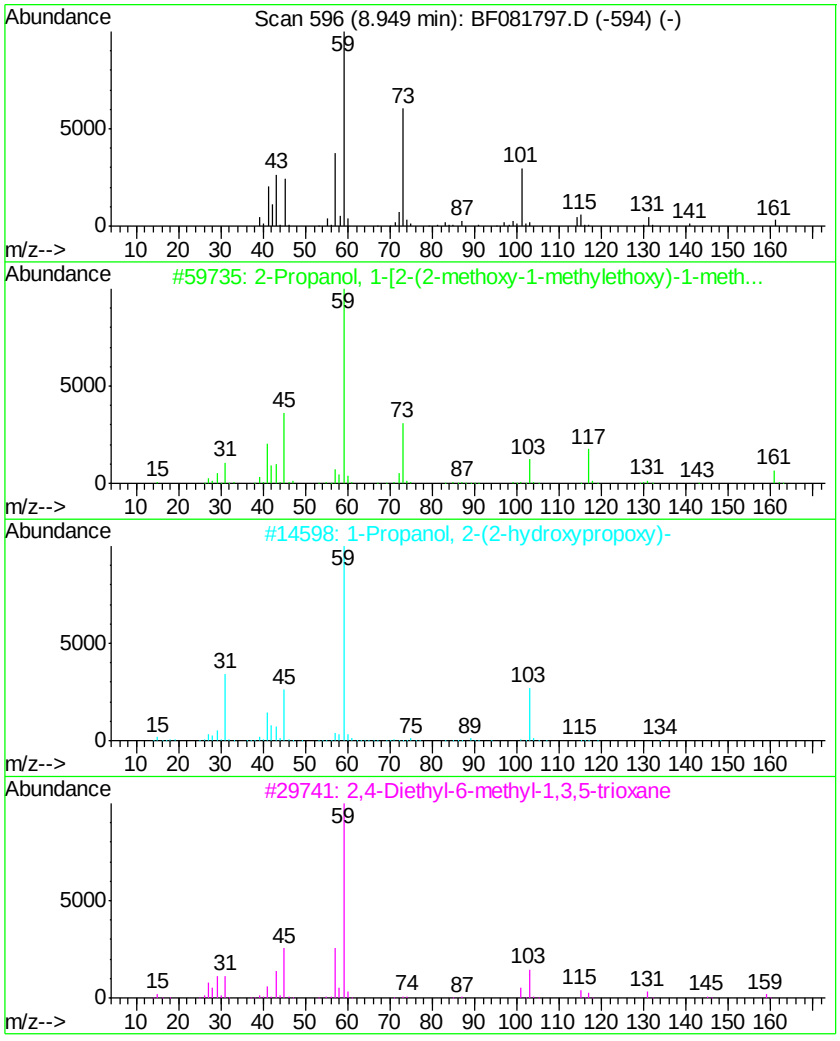
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

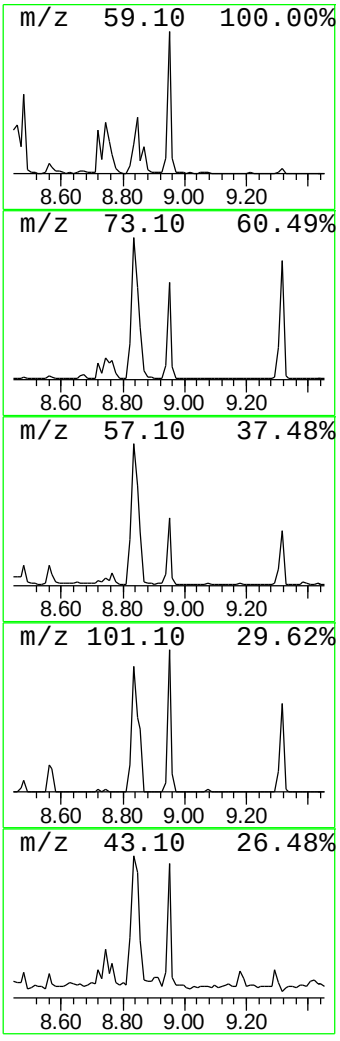
****

Peak Number 8 1-Propanol, 2-(2-hydroxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	4.04 ng	212270	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	53
4	2,5,8,11-Tetraoxatetradecan-13-o...	264	C13H28O5	020324-34-9	53
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	45





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

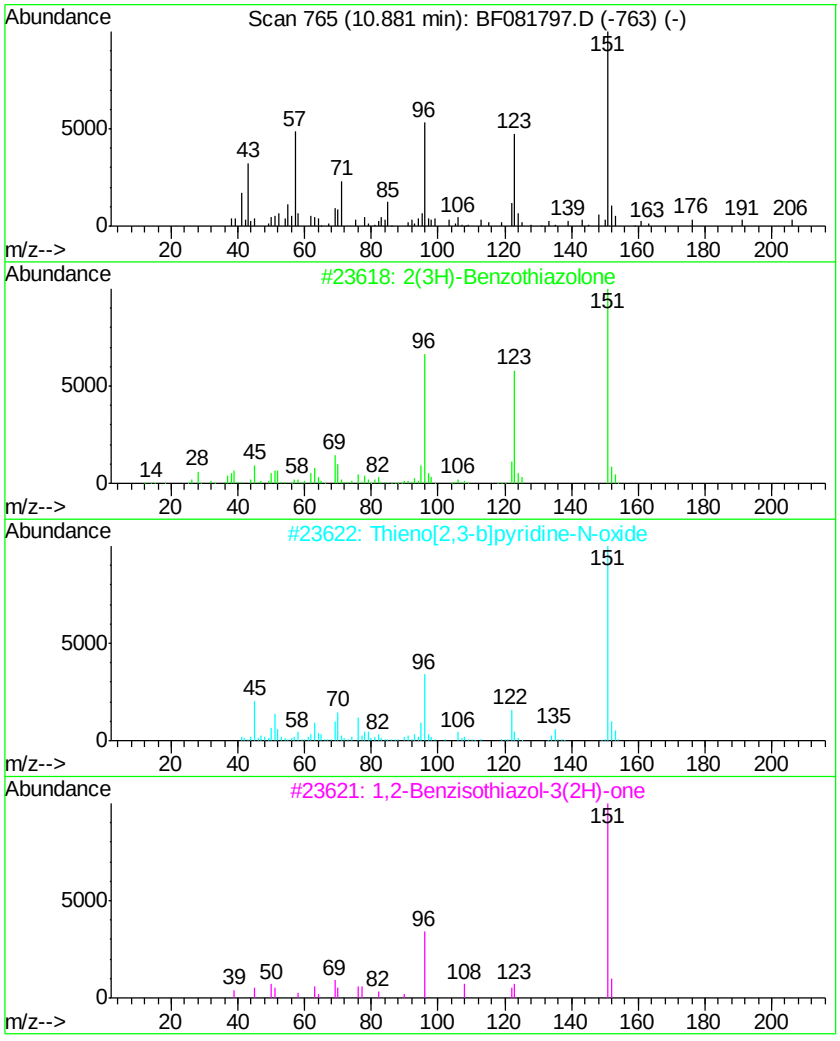
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

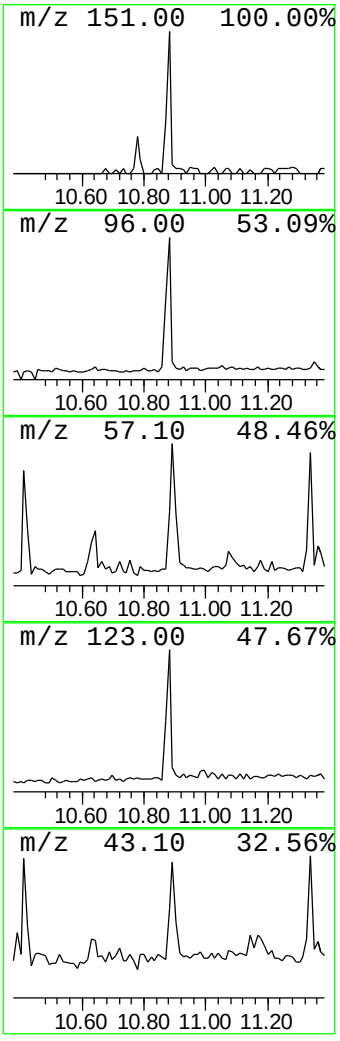
****

Peak Number 9 2(3H)-Benzothiazolone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.11 ng	108712	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	90
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	47
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	38
4	1H-Imidazo[4,5-b]pyridine-2-thiol	151	C6H5N3S	029448-81-5	38
5	1H-Isoindole-1,3(2H)-dione, 3a,4...	151	C8H9NO2	001469-48-3	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

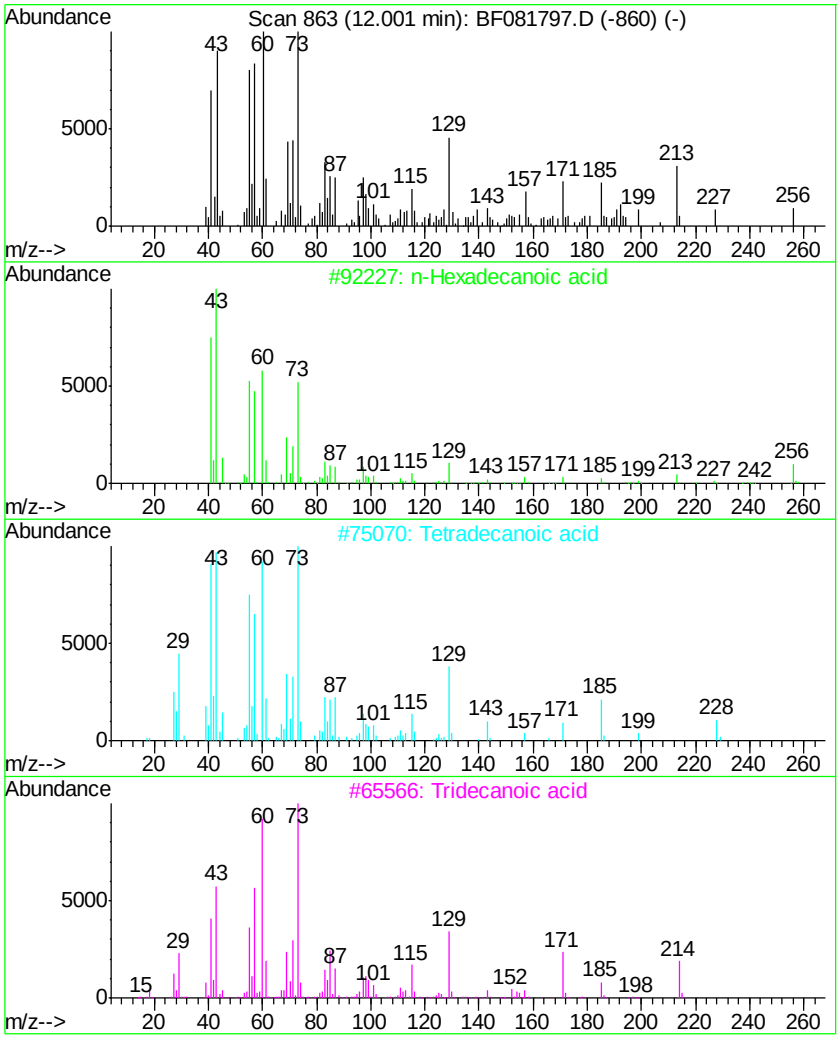
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

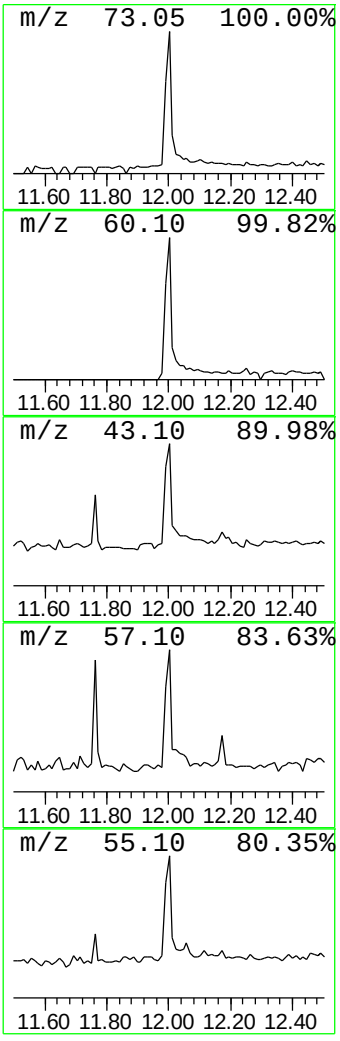
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	3.08 ng	158156	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092415\
Data File : BF081797.D
Acq On : 25 Sep 2015 9:40
Operator : UM/IZ
Sample : G3704-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5-9-15-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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
Propane, 1,1-dime...	2.22	6.1	ng	247123	1	6.95	815753	20.0
2-Pentanone, 4-hy...	5.14	10.8	ng	438589	1	6.95	815753	20.0
unknown6.72	6.72	72.7	ng	2964010	1	6.95	815753	20.0
2-t-Butyl-5-methy...	6.88	2.4	ng	97486	1	6.95	815753	20.0
2-Propanol, 1-[2-...	8.74	4.9	ng	255884	2	8.24	1050440	20.0
unknown8.33	8.83	11.4	ng	599726	2	8.24	1050440	20.0
1-Propanol, 2-(2-...	8.95	4.0	ng	212270	2	8.24	1050440	20.0
2(3H)-Benzothiazo...	10.88	2.1	ng	108712	4	11.48	1028480	20.0
n-Hexadecanoic acid	12.00	3.1	ng	158156	4	11.48	1028480	20.0