LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112316\
Data File : BF091309.D
Acq On : 24 Nov 2016 11:45
Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

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-BF112316.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	1.767	5	7	17	rVV	437182	856470	13.61%	1.429%
2	1.904	17	19	40	rVB	3578480	6290669	100.00%	10.496%
3	2.407	61	63	74	rVB	32108	74855	1.19%	0.125%
4	4.316	228	230	234	rBV	91927	114438	1.82%	0.191%
5	5.059	292	295	298	rBV	734199	799453	12.71%	1.334%
6	5.481	329	332	334	rBV	1837438	2438851	38.77%	4.069%
7	6.499	418	421	425	rBV	1687495	1658024	26.36%	2.766%
8	6.647	431	434	436	rBV	4358255	4265614	67.81%	7.117%
9	6.682	436	437	438	rVV	437065	387549	6.16%	0.647%
10	6.716	438	440	441	rVV	506372	448185	7.12%	0.748%
11	6.739	441	442	446	rVB	169939	218390	3.47%	0.364%
12	6.819	446	449	451	rBV	2615327	3118042	49.57%	5.202%
13	6.876	452	454	456	rBV	1999562	2314866	36.80%	3.862%
14	6.910	456	457	459	rVB	828607	623372	9.91%	1.040%
15	7.036	465	468	470	rVB	3824500	4009153	63.73%	6.689%
16	7.447	498	504	506	rBV	3273153	4183593	66.50%	6.980%
17	8.167	564	567	569	rBV	3348837	3087350	49.08%	5.151%
18	8.659	608	610	611	rBV	185861	168868	2.68%	0.282%
19	8.705	611	614	617	rVV	408210	682100	10.84%	1.138%
20	8.773	617	620	627	rVB2	1239756	2490169	39.59%	4.155%
21	8.888	627	630	632	rBV	730193	658055	10.46%	1.098%
22	9.242	658	661	664	rBV	4914127	5618677	89.32%	9.375%
23	9.653	692	697	701	rBV	186395	255555	4.06%	0.426%
24	9.722	701	703	708	rVB	69284	88129	1.40%	0.147%
25	9.916	718	720	723	rVB	2402948	2722736	43.28%	4.543%
26	10.145	736	740	741	rBV	46646	68310	1.09%	0.114%
27	10.705	786	789	791	rBV	1331515	1386515	22.04%	2.313%
28	11.402	847	850	852	rVB	2798201	2423472	38.52%	4.043%
29	12.991	986	989	991	rBV	4711213	4458613	70.88%	7.439%
30	14.031	1078	1080	1083	rBV	1758701	2231404	35.47%	3.723%
31	14.900	1154	1156	1158	rBV	74880	79574	1.26%	0.133%
32	15.482	1203	1207	1209	rBV	1180921	1714516	27.25%	2.861%

LSC Area Percent Report

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Data File : BF091309.D
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Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
MW-4

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-BF112316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

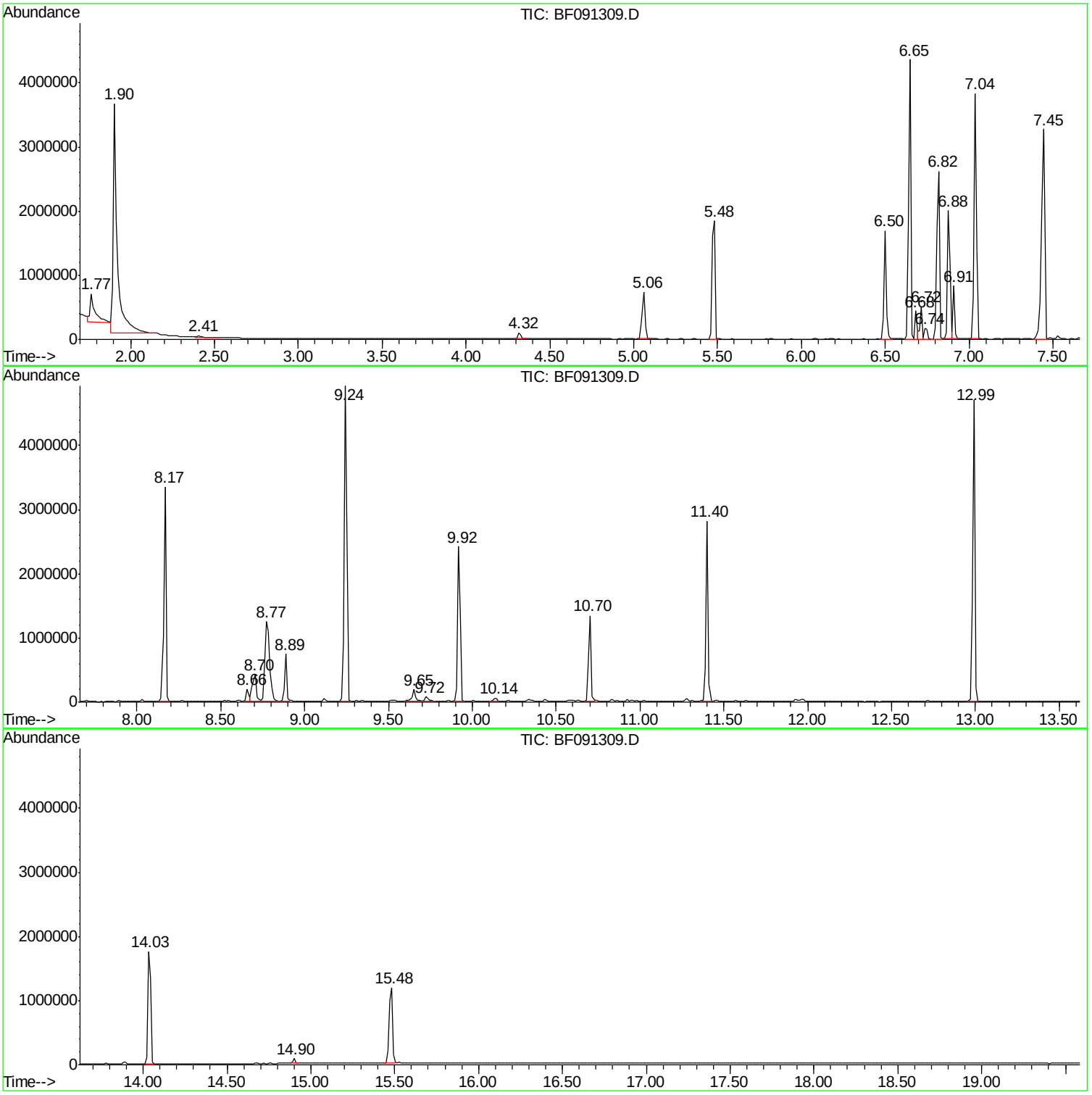
Sum of corrected areas: 59935567

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112316\
Data File : BF091309.D
Acq On : 24 Nov 2016 11:45
Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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\BF112316\
Data File : BF091309.D
Acq On : 24 Nov 2016 11:45
Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

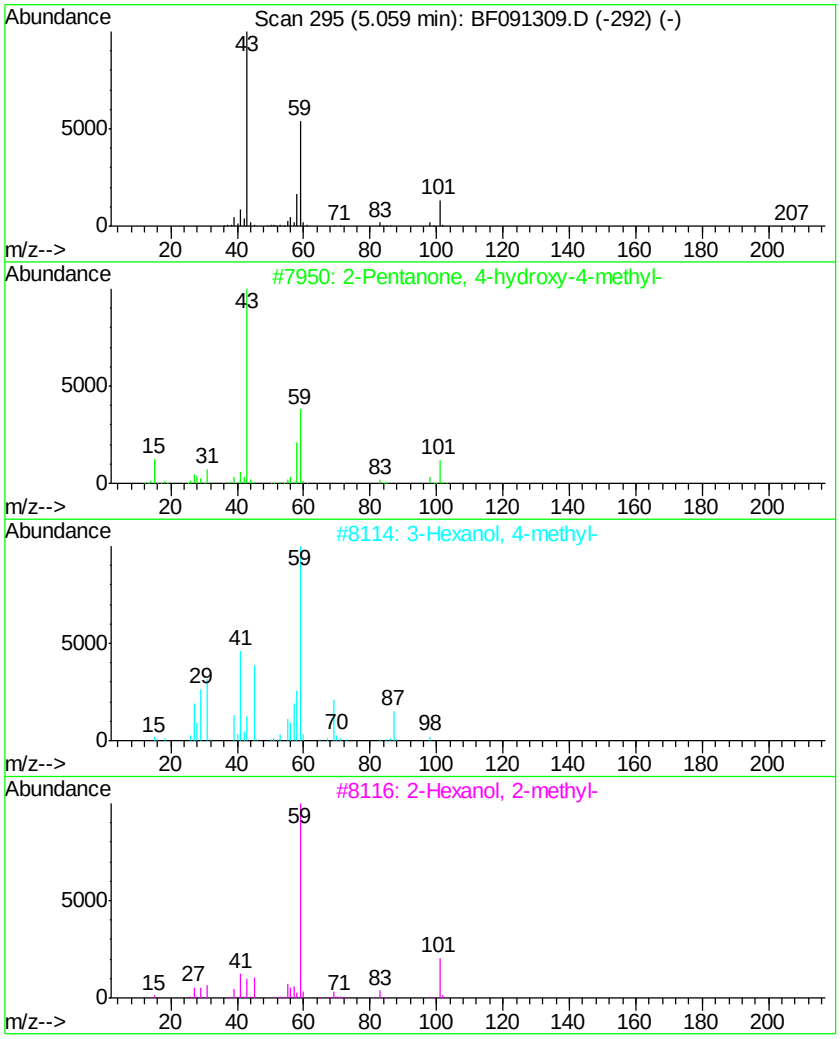
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

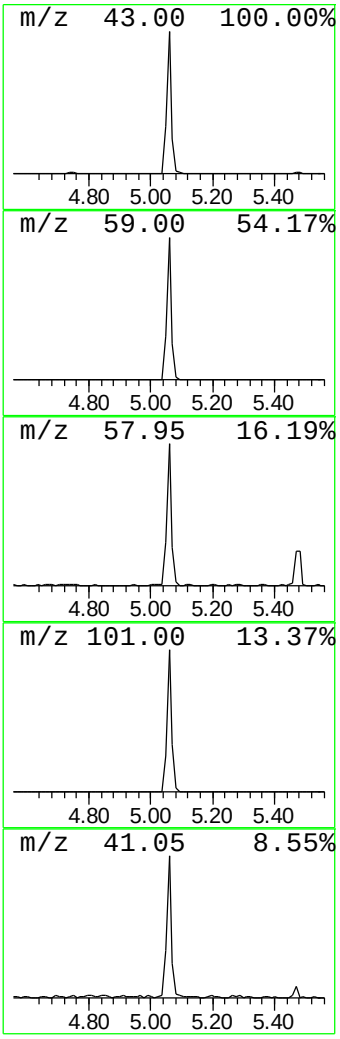
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	6.91 ng	799453	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112316\
Data File : BF091309.D
Acq On : 24 Nov 2016 11:45
Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

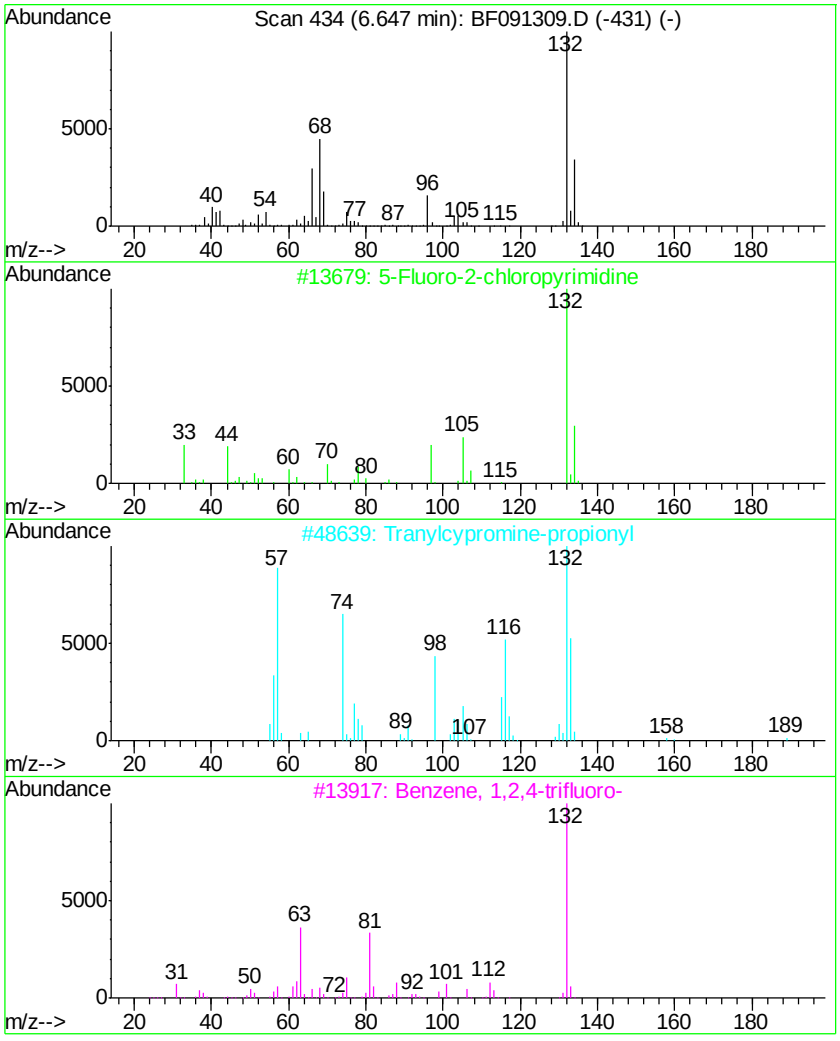
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

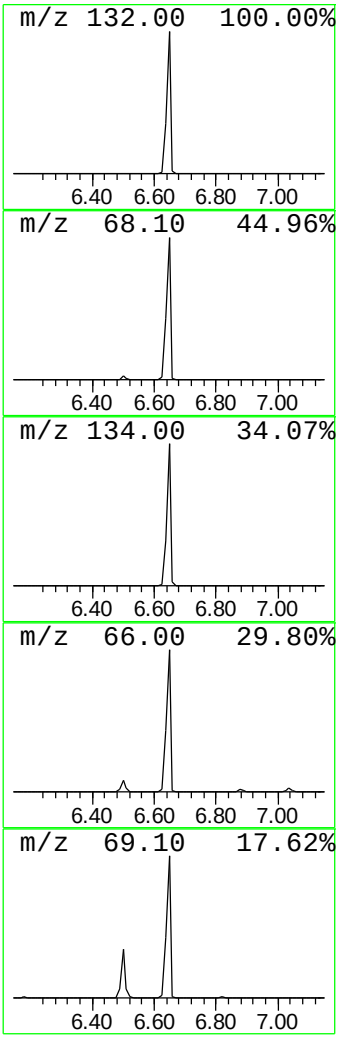
****

Peak Number 4 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	36.85 ng	4265610	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112316\
Data File : BF091309.D
Acq On : 24 Nov 2016 11:45
Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

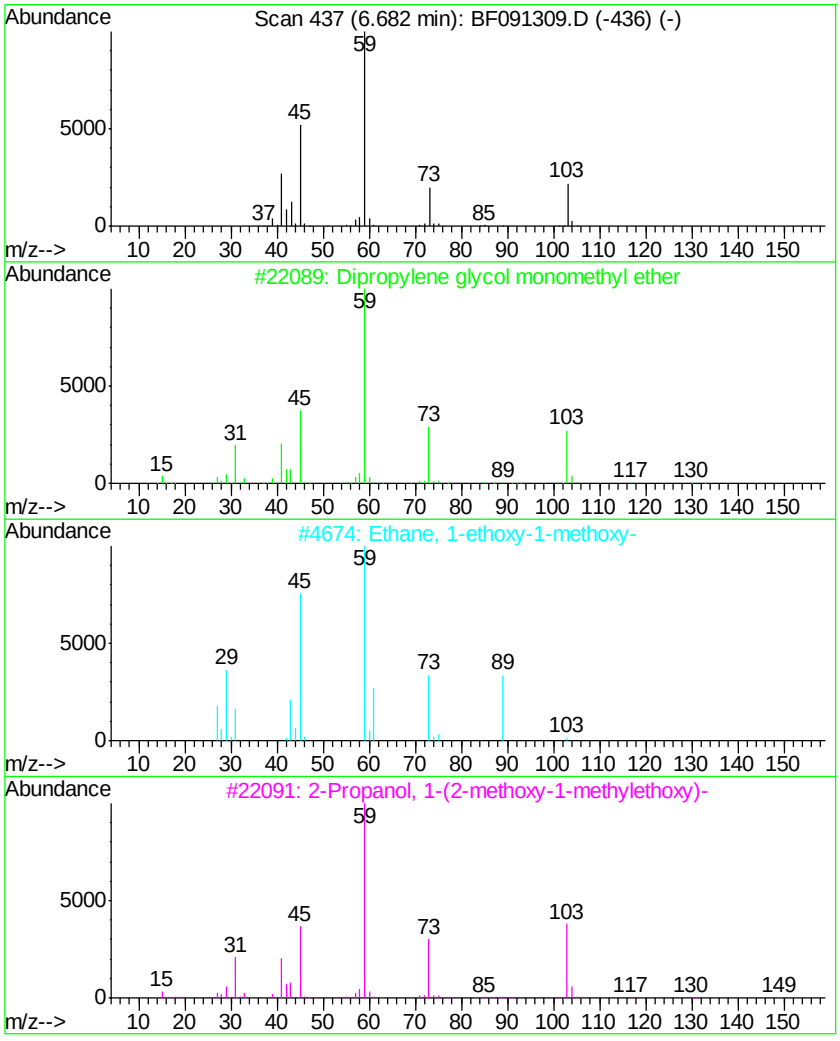
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

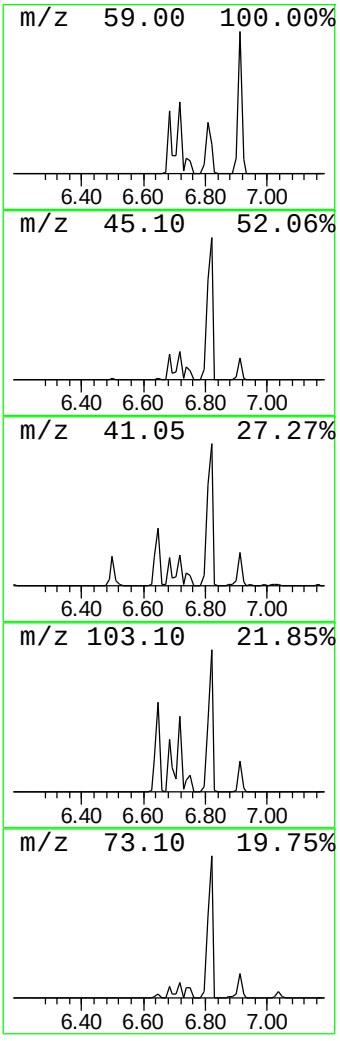
****

Peak Number 5 Dipropylene glycol monometh... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	3.35 ng	387549	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64
3	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
5	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	50





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Operator : UM/SJ
Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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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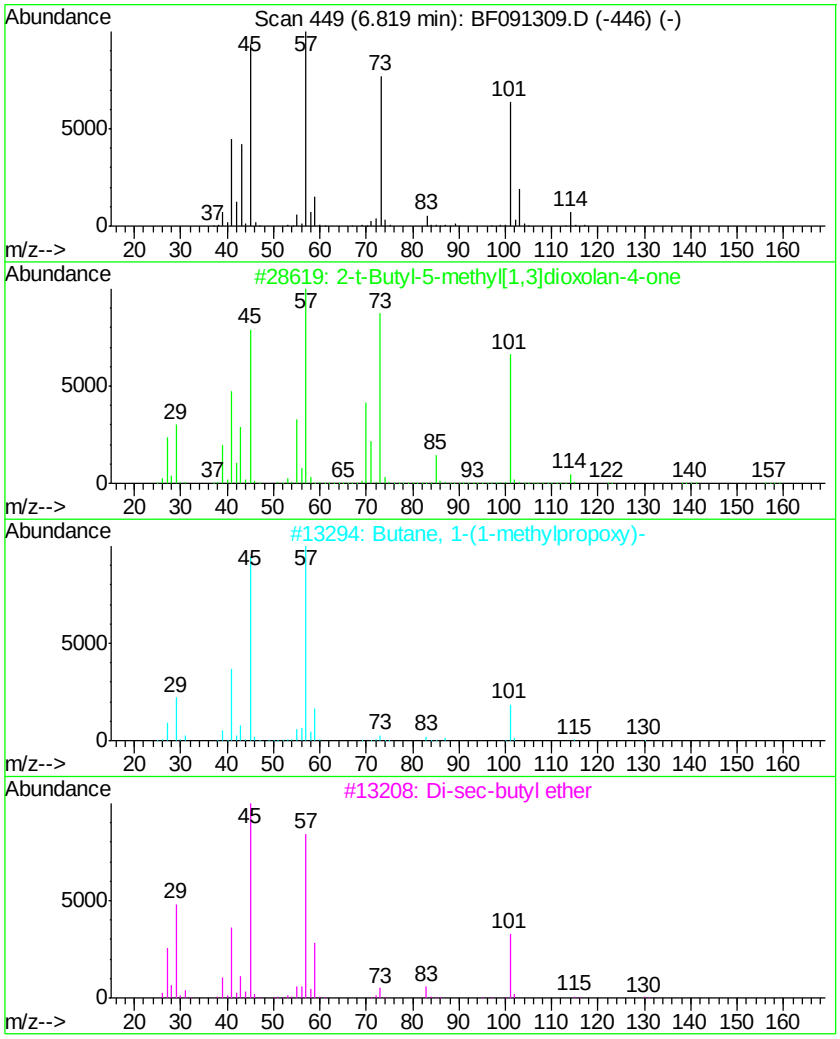
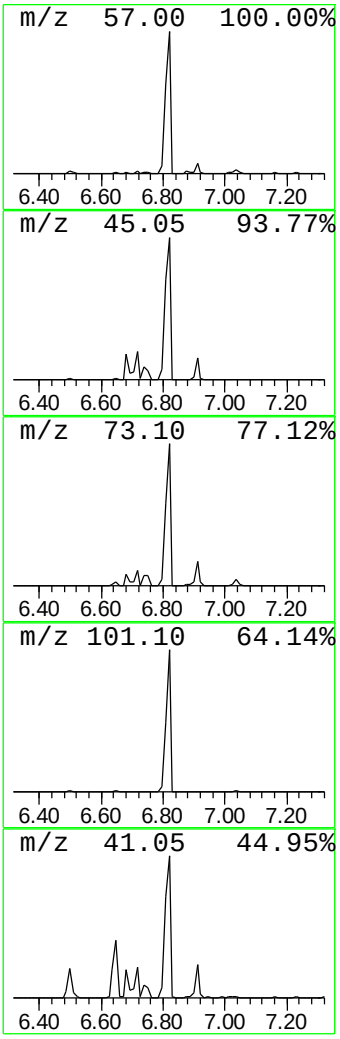
Peak Number 7 2-t-Butyl-5-methyl[1,3]diox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	26.94 ng	3118040	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	56
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	45
4	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	36
5	2-Oxopentanedioic acid	146	C5H6O5	000328-50-7	36





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Sample : H5721-02
Misc :
ALS Vial : 30 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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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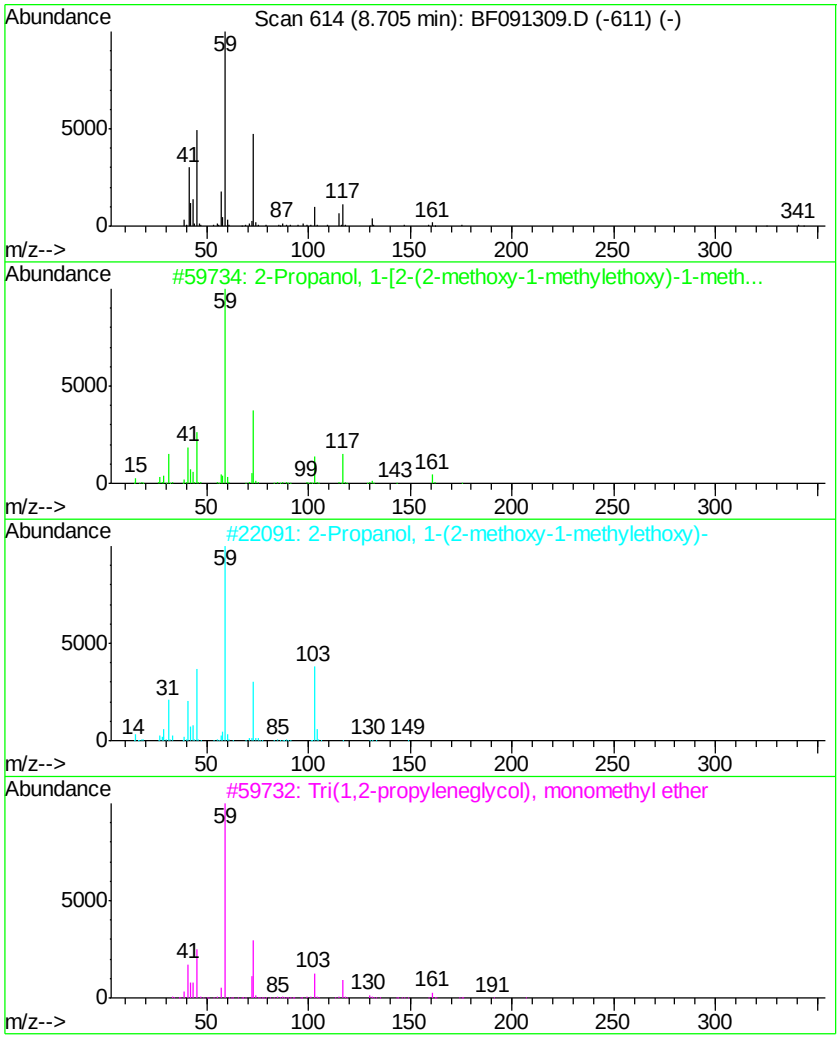
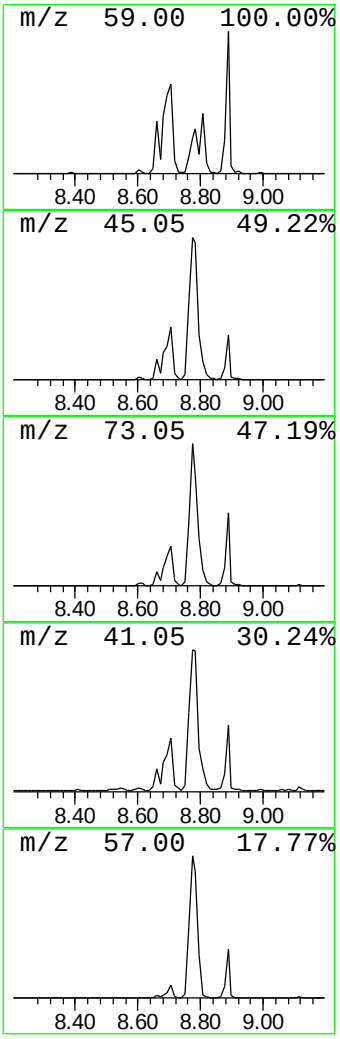
Peak Number 9 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	4.42 ng	682100	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	56
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	56
3	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	50
4	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	50
5	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	50





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Sample : H5721-02
Misc :
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Instrument : BNA_F
ClientSampleId : MW-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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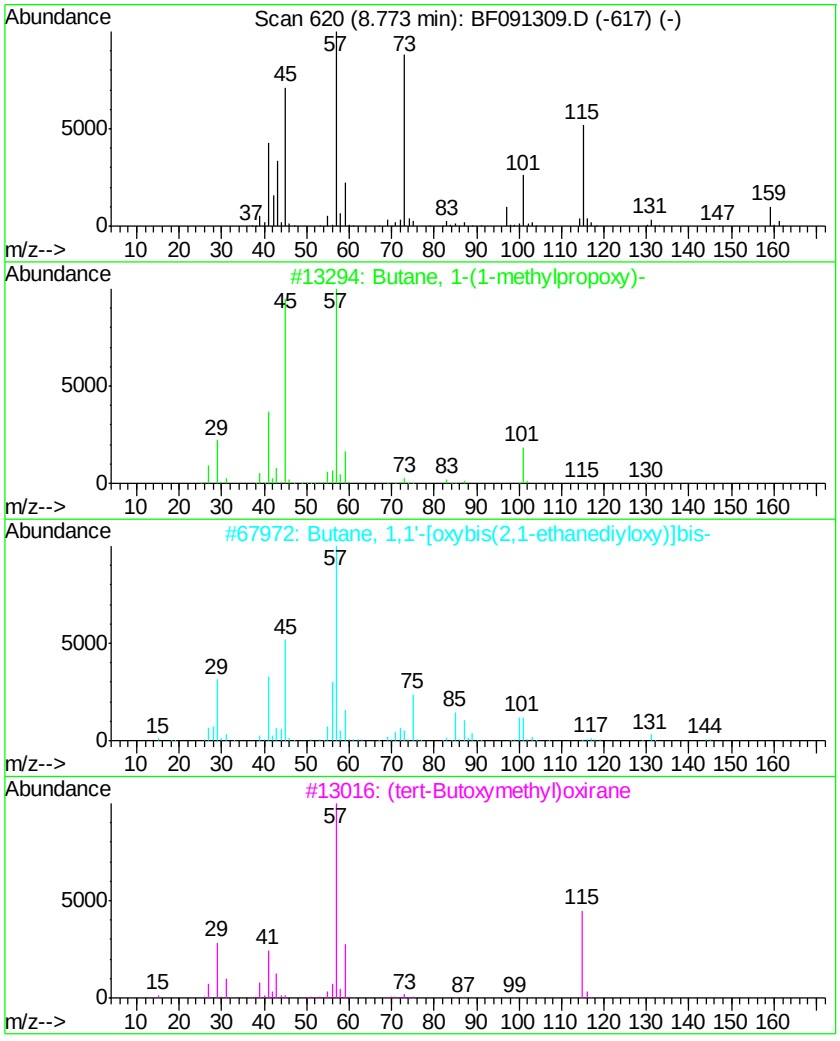
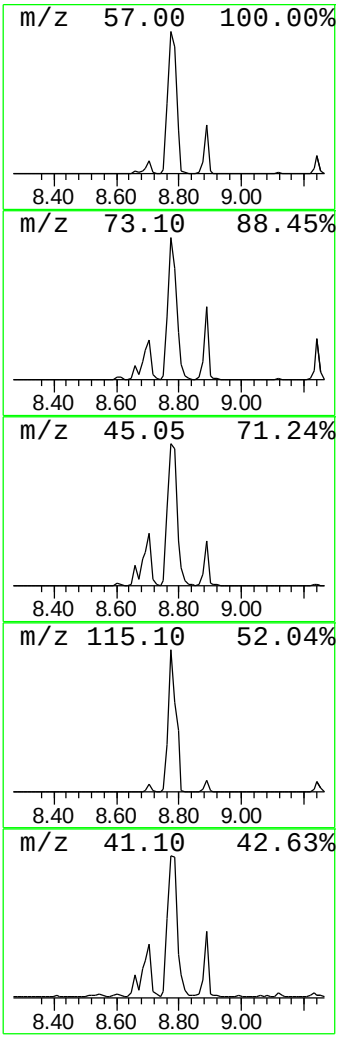
Peak Number 10 unknown8.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	16.13 ng	2490170	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	35
2	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	32
3	(tert-Butoxymethyl)oxirane	130	C7H14O2	007665-72-7	25
4	Isobutyl isothiocyanate	115	C5H9NS	000591-82-2	22
5	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	22





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.06	6.9	ng	799453	1	6.88	2314870	20.0
unknown6.65	6.65	36.9	ng	4265610	1	6.88	2314870	20.0
Dipropylene glyco...	6.68	3.4	ng	387549	1	6.88	2314870	20.0
2-t-Butyl-5-methy...	6.82	26.9	ng	3118040	1	6.88	2314870	20.0
2-Propanol, 1-[2-...	8.70	4.4	ng	682100	2	8.17	3087350	20.0
unknown8.77	8.77	16.1	ng	2490170	2	8.17	3087350	20.0