LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092693.D
Acq On : 31 Jan 2017 20:52
Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

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-BF013017.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	5.127	263	266	268	rBV	533333	759550	1.75%	0.715%
2	5.550	301	303	310	rVB	1646822	2567455	5.92%	2.416%
3	6.590	391	394	398	rBV	394884	1147703	2.65%	1.080%
4	6.716	402	405	413	rVB	2650918	4935818	11.39%	4.645%
5	6.945	423	425	427	rBV	1249281	1124428	2.59%	1.058%
6	7.105	436	439	441	rBV	3715005	3792590	8.75%	3.569%
7	7.516	471	475	477	rBV	3111311	3574283	8.25%	3.364%
8	7.859	502	505	506	rBV	630929	712889	1.65%	0.671%
9	7.893	506	508	513	rVV2	612084	1420462	3.28%	1.337%
10	8.145	525	530	535	rBV2	211359	543820	1.25%	0.512%
11	8.236	535	538	543	rVB	1559807	1521912	3.51%	1.432%
12	8.522	554	563	564	rBV3	8372958	43336686	100.00%	40.784%
13	8.625	568	572	575	rVB	7787982	16783229	38.73%	15.794%
14	9.322	630	633	635	rVV	5159569	5313805	12.26%	5.001%
15	9.996	690	692	695	rVB	1790453	1619500	3.74%	1.524%
16	10.796	759	762	764	rVV	2603915	3178774	7.34%	2.991%
17	11.482	820	822	825	rBV	1128197	1459836	3.37%	1.374%
18	11.665	833	838	840	rBV2	271195	575287	1.33%	0.541%
19	13.071	958	961	964	rBV	3460974	5124046	11.82%	4.822%
20	13.539	1000	1002	1005	rVB	718496	741418	1.71%	0.698%
21	13.631	1008	1010	1012	rBV	2297975	2133723	4.92%	2.008%
22	13.848	1026	1029	1031	rBV	1311472	1145433	2.64%	1.078%
23	14.122	1049	1053	1056	rBV	1606209	1561510	3.60%	1.470%
24	15.597	1178	1182	1188	rVB	770600	1186136	2.74%	1.116%

Sum of corrected areas: 106260293

LSC Report - Integrated Chromatogram

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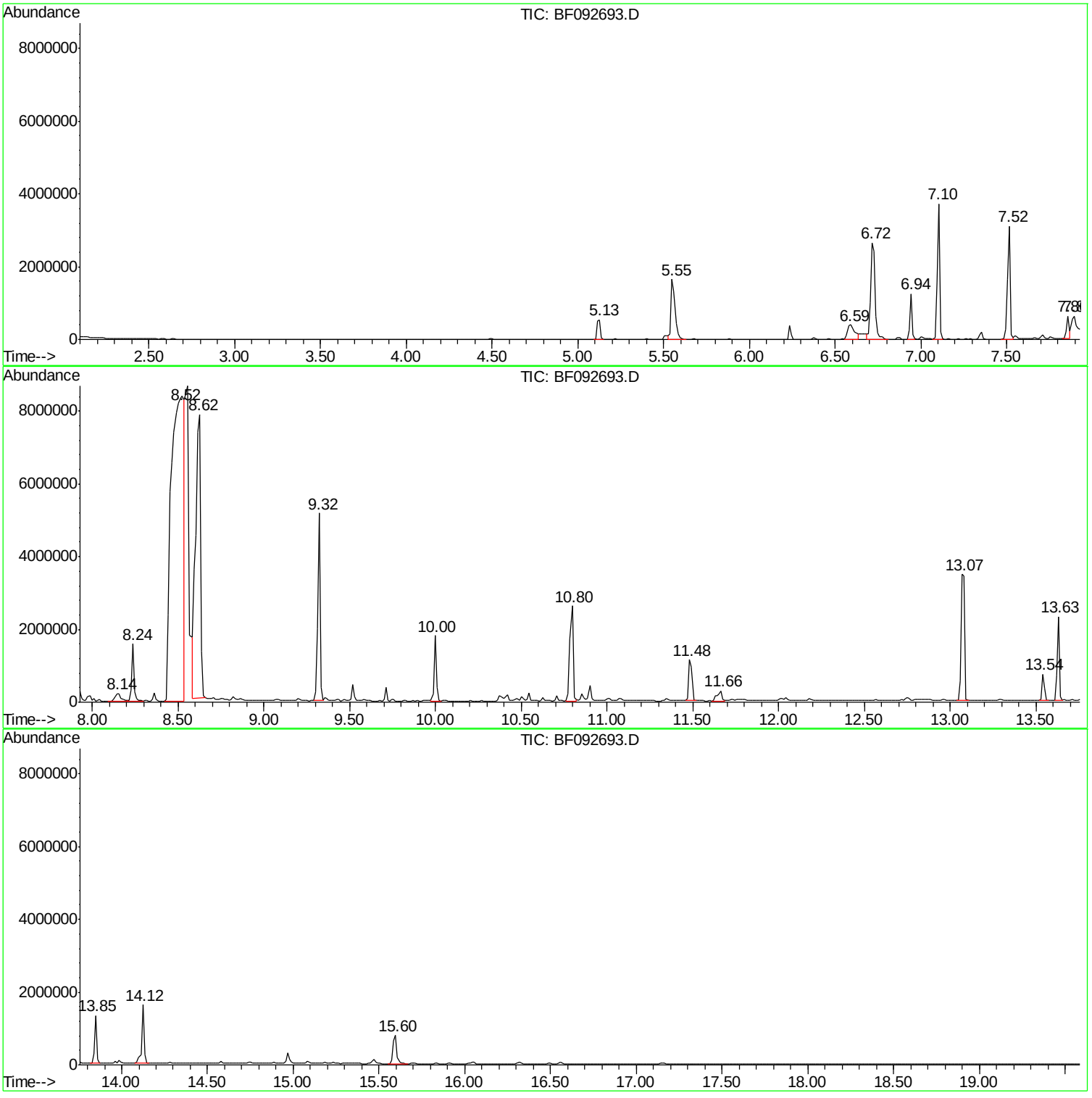
Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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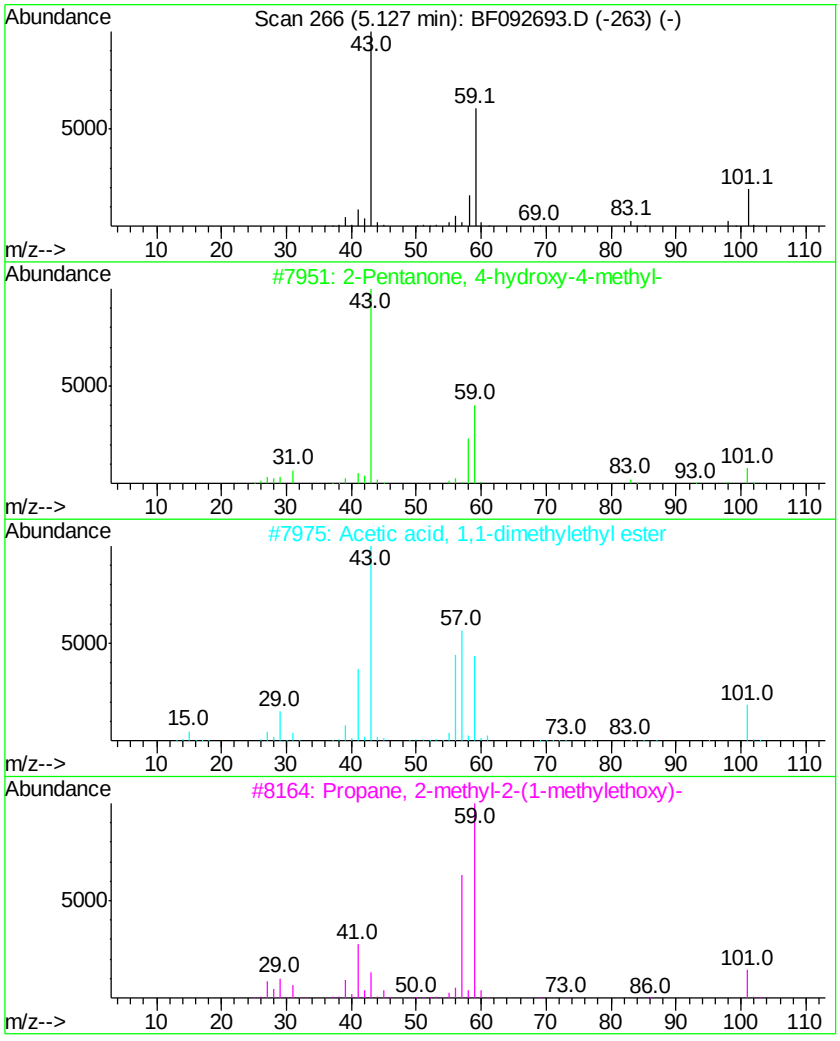
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

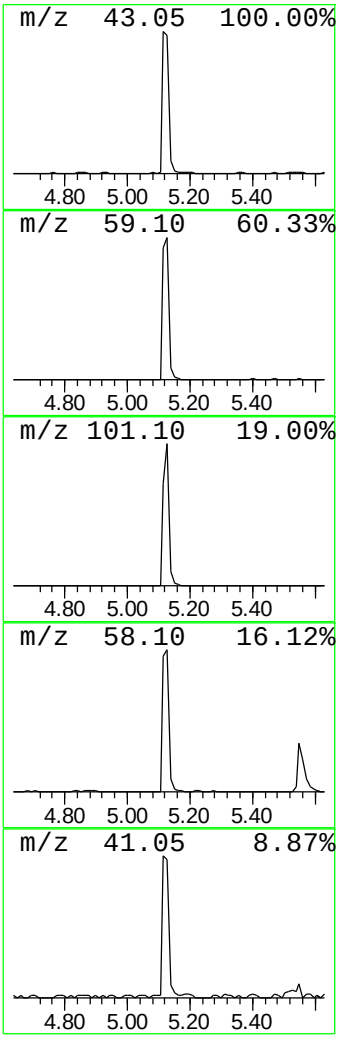
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	13.51 ng	759550	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : MH-6

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TIC Integration Parameters: LSCINT.P

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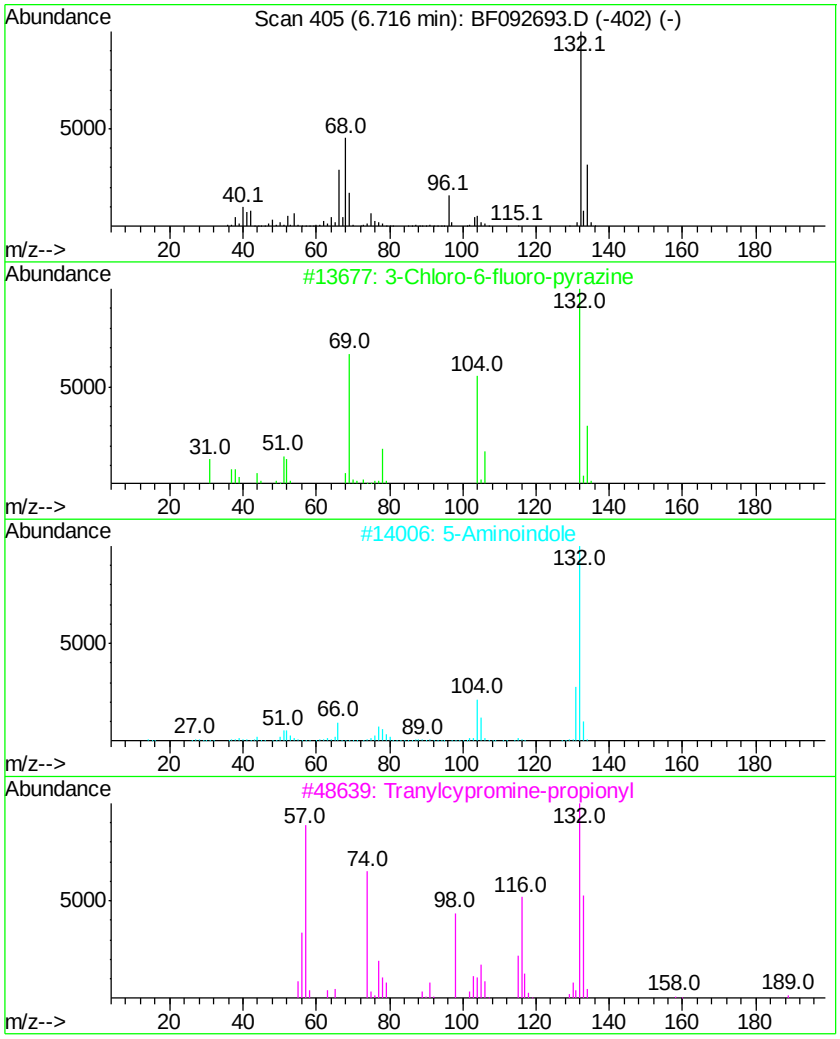
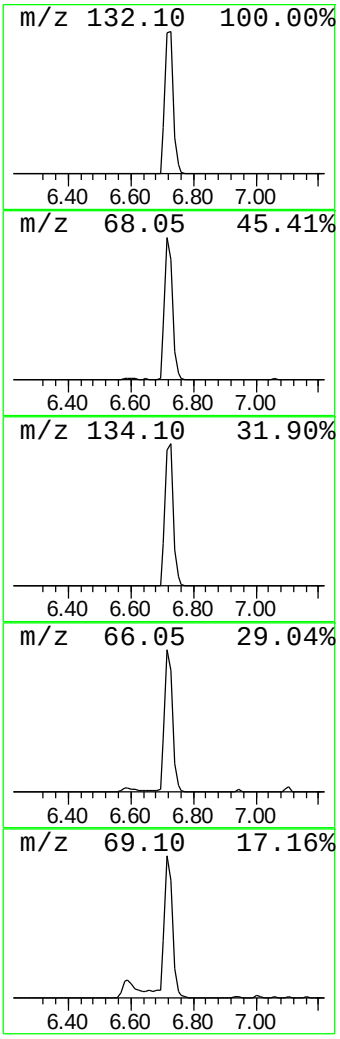
Peak Number 2 unknown6.72 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	87.79 ng	4935820	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Acq On : 31 Jan 2017 20:52
Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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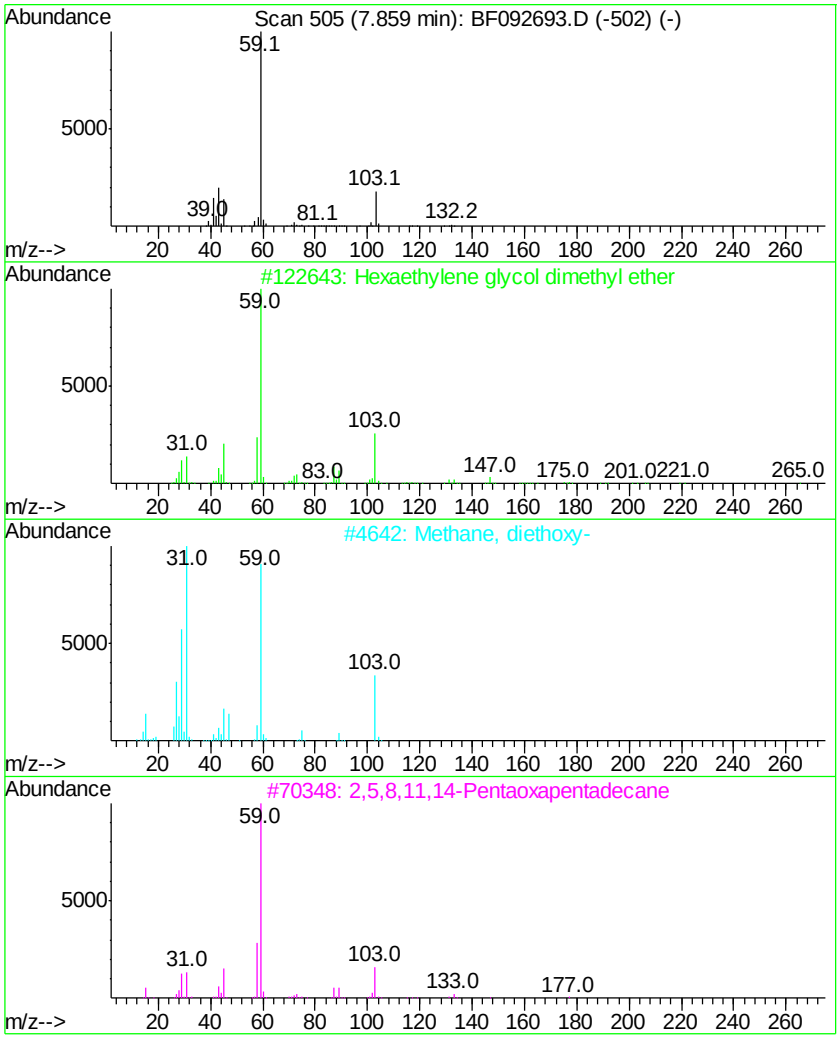
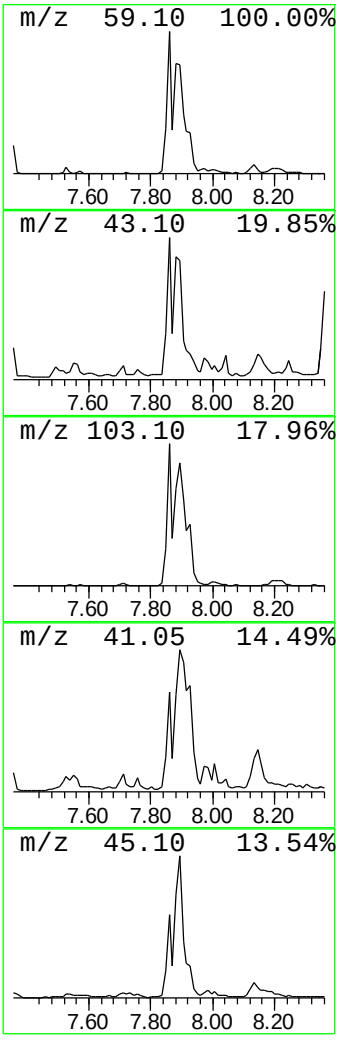
Peak Number 4 Hexaethylene glycol dimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	9.37 ng	712889	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	78
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	78
3	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	78
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72





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Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

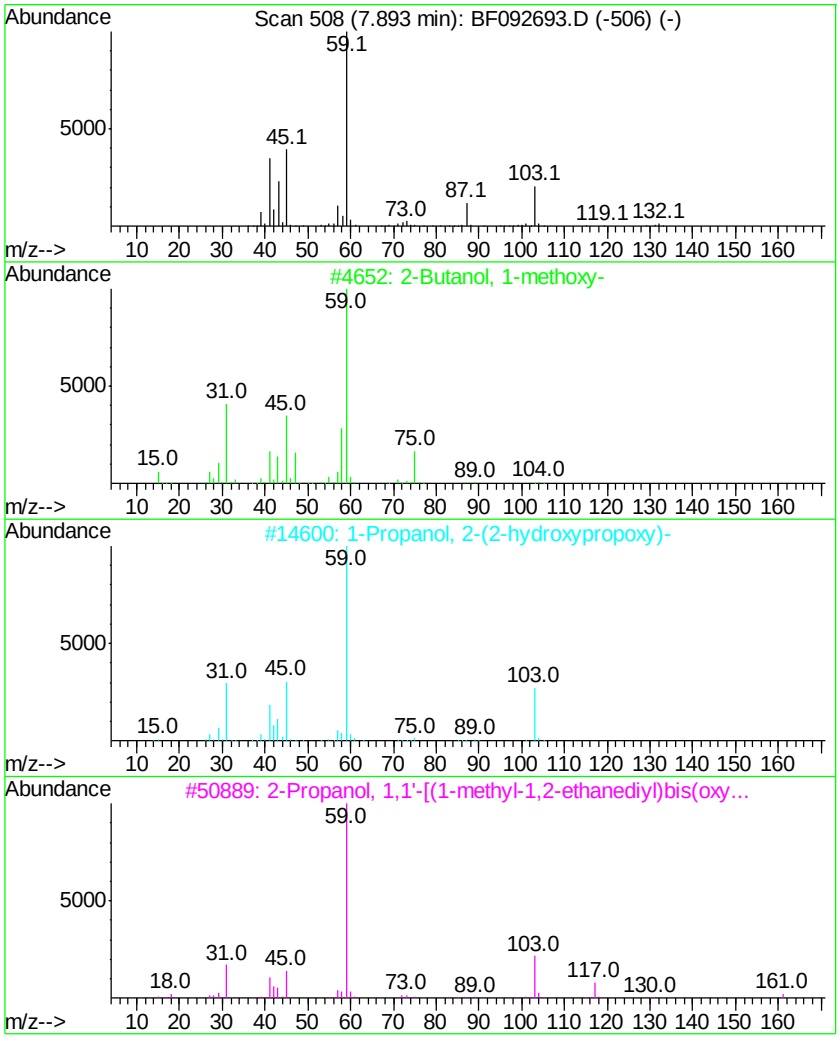
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

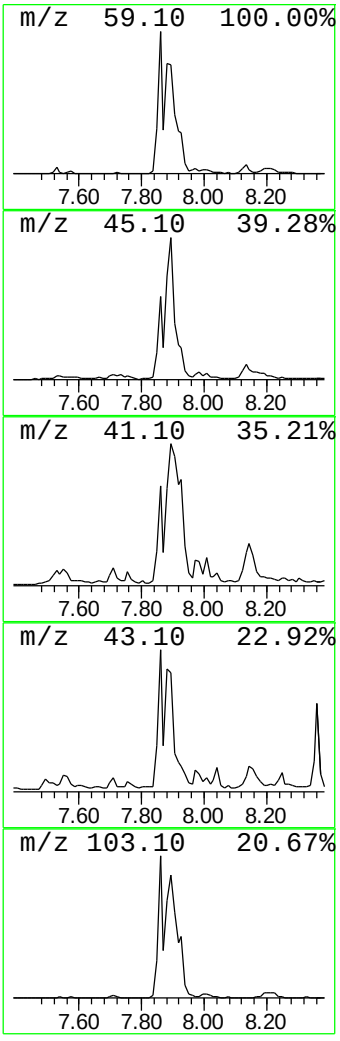
****

Peak Number 5 2-Butanol, 1-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.89	18.67 ng	1420460	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	59
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53
4	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	53
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

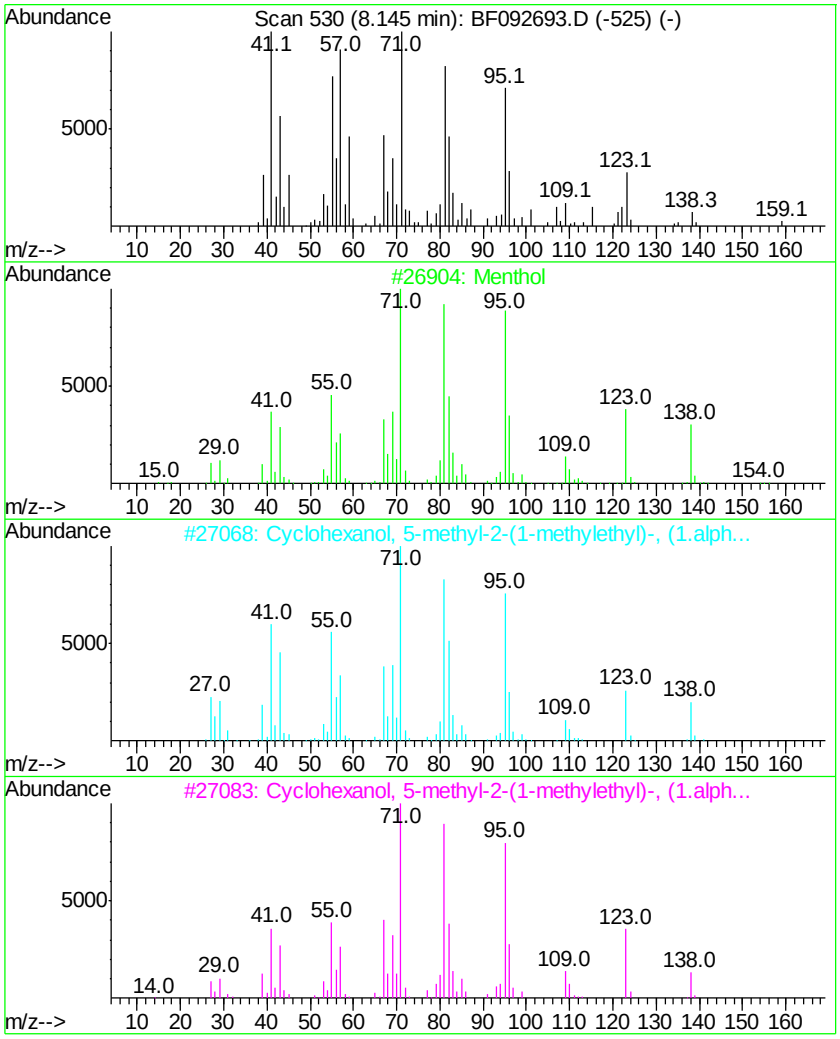
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

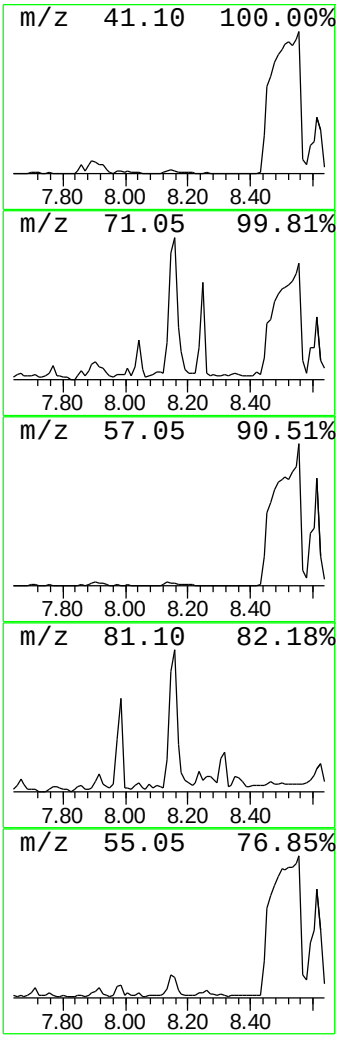
****

Peak Number 6 Menthol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.14	7.15 ng	543820	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Menthol	156	C10H20O	001490-04-6	80
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000089-78-1	80
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	72
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-51-5	72
5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-60-2	64





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

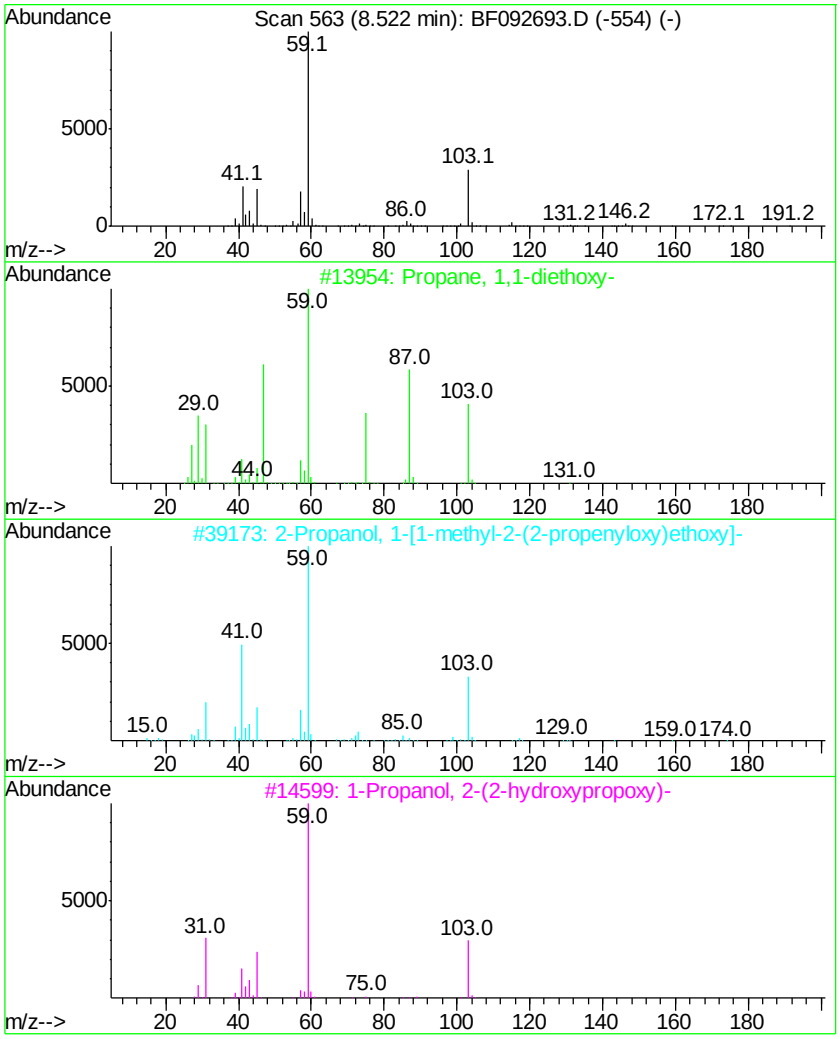
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

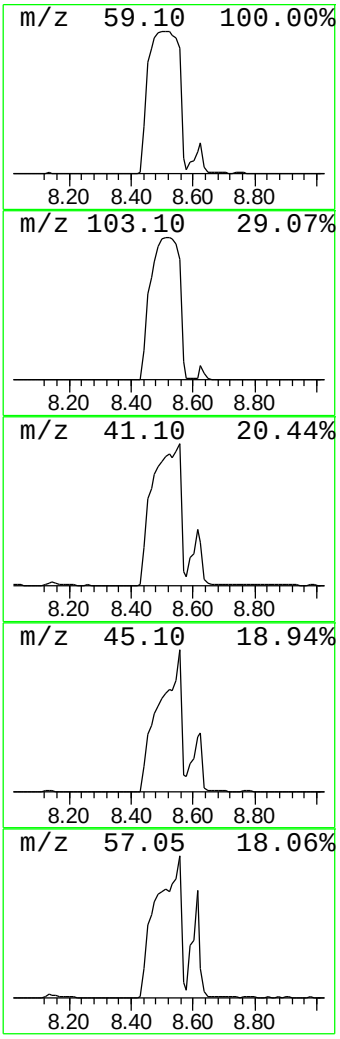
****

Peak Number 7 Propane, 1,1-diethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	569.50 ng	43336700	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	78
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	72
5	Dipropylene glycol	134	C6H14O3	025265-71-8	64





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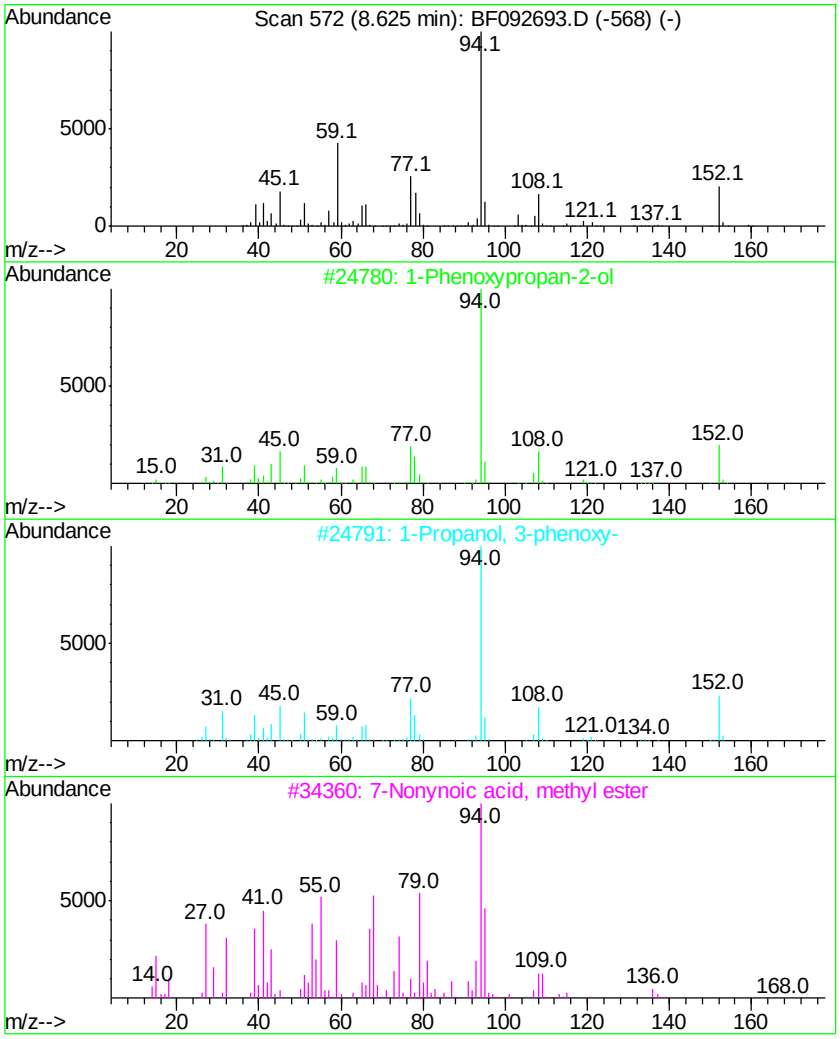
TIC Integration Parameters: LSCINT.P

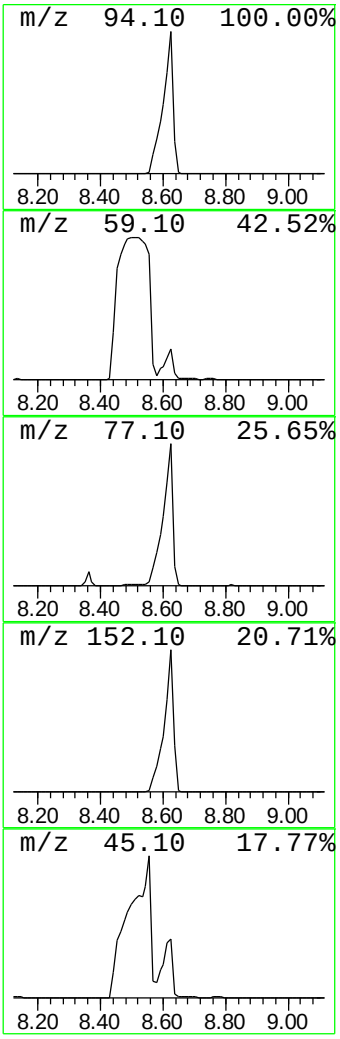
****

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	220.56 ng	16783200	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	81
3	7-Nonynoic acid, methyl ester	168	C10H16O2	020731-18-4	50
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	47
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	43





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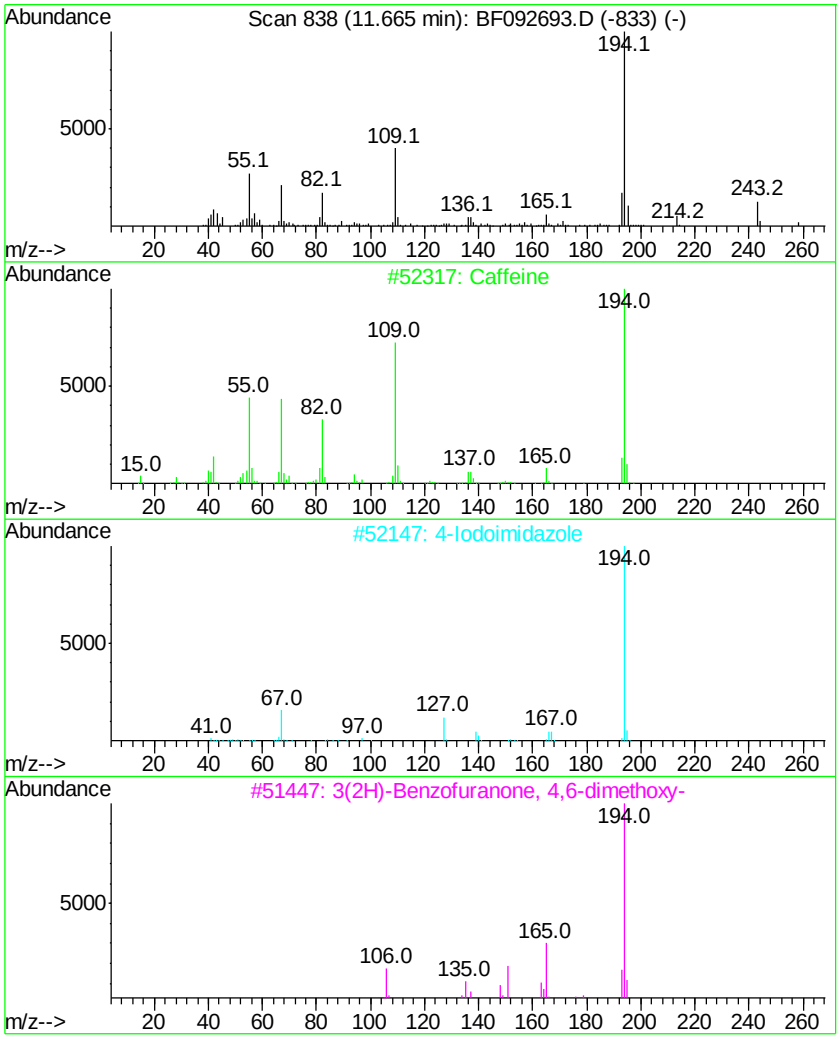
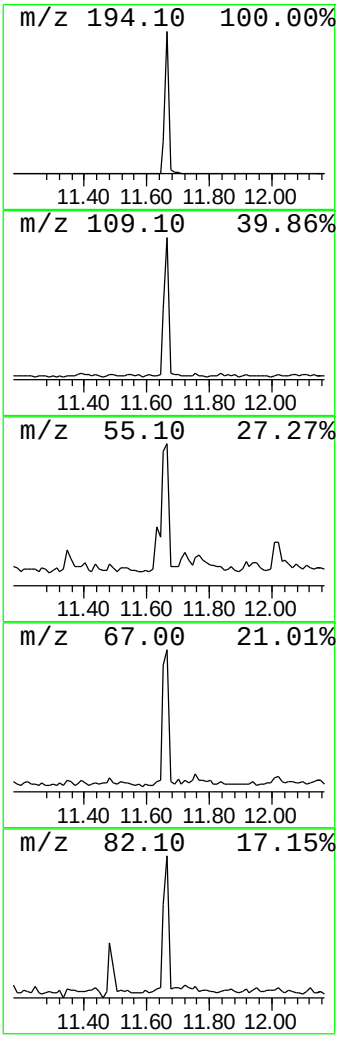
Peak Number 9 Caffeine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	7.88 ng	575287	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	95
2	4-Iodoimidazole	194	C3H3IN2	071759-89-2	47
3	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	47
4	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	47
5	1H-Benzimidazole, 2-phenyl-	194	C13H10N2	000716-79-0	43





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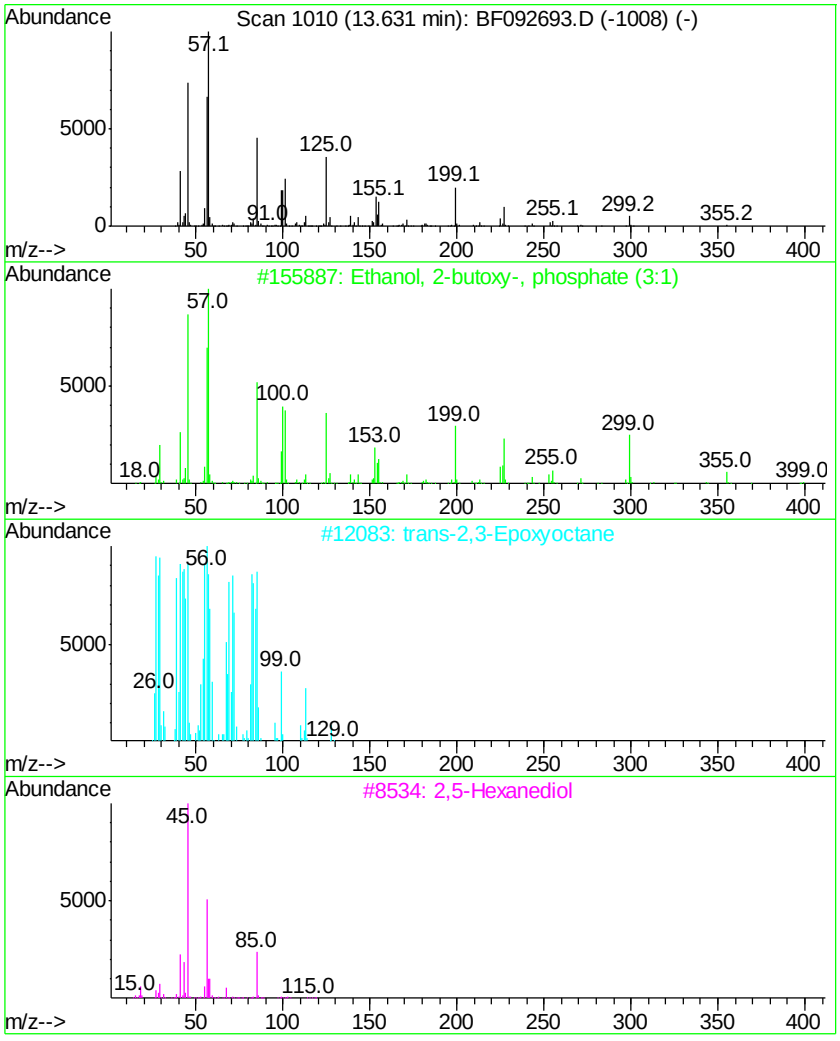
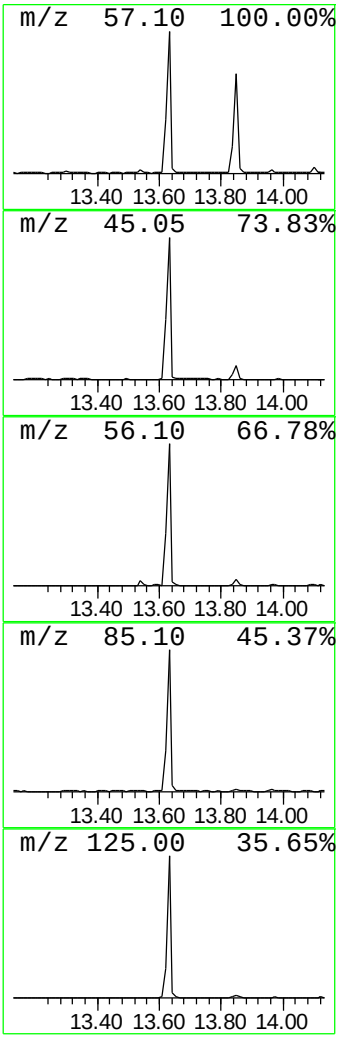
****

Peak Number 10 Ethanol, 2-butoxy-, phospha... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	27.33 ng	2133720	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	83
2	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47
3	2,5-Hexanediol	118	C6H14O2	002935-44-6	38
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	27
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	27





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Operator : SJ/MA
Sample : I1594-01
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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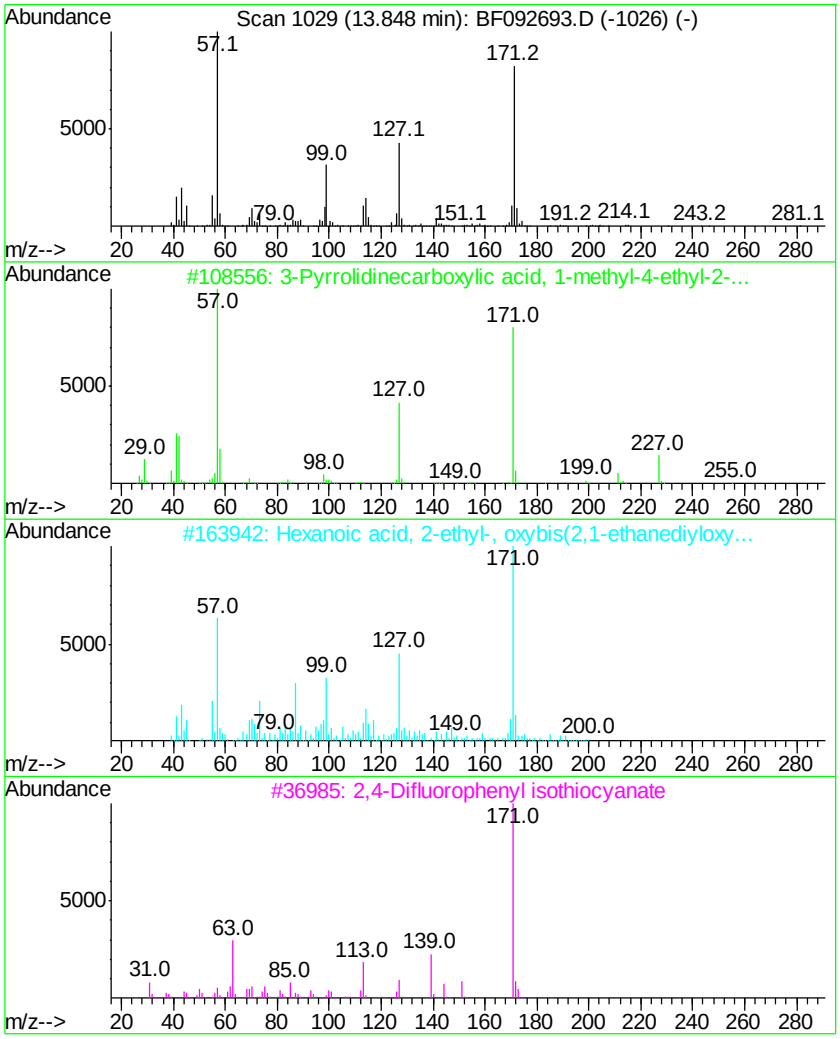
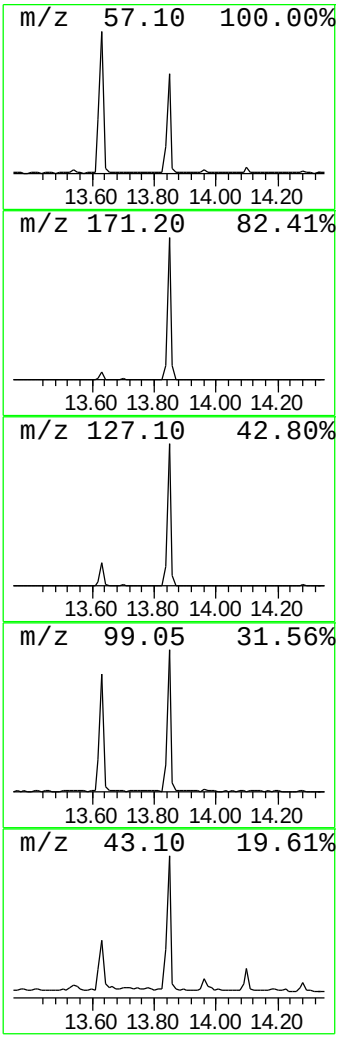
Peak Number 11 3-Pyrrolidinecarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	14.67 ng	1145430	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyrrolidinecarboxylic acid, 1-...	284	C15H28N2O3	1000196-95-3	53
2	Hexanoic acid, 2-ethyl-, oxybis(...	446	C24H46O7	018268-70-7	40
3	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	35
4	4-Fluoro-5-amino veratrole	171	C8H10FNO2	000397-75-1	32
5	1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013117\
Data File : BF092693.D
Acq On : 31 Jan 2017 20:52
Operator : SJ/MA
Sample : I1594-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
2-Pentanone, 4-hy...	5.13	13.5	ng	759550	1	6.94	1124430	20.0
unknown6.72	6.72	87.8	ng	4935820	1	6.94	1124430	20.0
Hexaethylene glyc...	7.86	9.4	ng	712889	2	8.24	1521910	20.0
2-Butanol, 1-meth...	7.89	18.7	ng	1420460	2	8.24	1521910	20.0
Menthol	8.14	7.2	ng	543820	2	8.24	1521910	20.0
Propane, 1,1-diet...	8.52	569.5	ng	43336700	2	8.24	1521910	20.0
1-Phenoxypropan-2-ol	8.62	220.6	ng	16783200	2	8.24	1521910	20.0
Caffeine	11.67	7.9	ng	575287	4	11.48	1459840	20.0
Ethanol, 2-butoxy...	13.63	27.3	ng	2133720	5	14.12	1561510	20.0
3-Pyrrolidinecarb...	13.85	14.7	ng	1145430	5	14.12	1561510	20.0