LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF030617\
Data File : BF093401.D
Acq On : 6 Mar 2017 15:28
Operator : SJ/MA
Sample : I2076-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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	1.978	6	8	18	rVB	89896	180511	3.15%	0.367%
2	4.253	204	207	220	rBV	119514	246898	4.30%	0.502%
3	4.927	264	266	277	rBV	667094	1320634	23.02%	2.686%
4	5.373	302	305	307	rBV	4430149	5400240	94.15%	10.984%
5	6.425	394	397	405	rBV	4611883	5575404	97.20%	11.340%
6	6.539	405	407	410	rBV	4380218	4763105	83.04%	9.688%
7	6.767	425	427	430	rBV	1237558	1116292	19.46%	2.270%
8	6.927	438	441	443	rBV	4180390	4121515	71.85%	8.383%
9	7.339	475	477	480	rBV	2681983	3471163	60.52%	7.060%
10	8.059	537	540	542	rBV	1340334	1423202	24.81%	2.895%
11	9.133	631	634	636	rBV	5392833	5735969	100.00%	11.667%
12	9.533	666	669	671	rBV	275261	338655	5.90%	0.689%
13	9.739	684	687	690	rBV	81702	164670	2.87%	0.335%
14	9.808	690	693	695	rVB	1645172	1600868	27.91%	3.256%
15	10.231	726	730	732	rBV	58336	83256	1.45%	0.169%
16	10.596	759	762	765	rBV2	2428183	3073094	53.58%	6.251%
17	10.711	770	772	776	rVB	87518	121363	2.12%	0.247%
18	11.156	808	811	812	rBV	66740	62769	1.09%	0.128%
19	11.294	820	823	825	rBV	1588491	1597741	27.85%	3.250%
20	12.882	959	962	964	rBV	4694248	5642642	98.37%	11.477%
21	13.762	1037	1039	1045	rBV	72808	125027	2.18%	0.254%
22	13.934	1051	1054	1056	rBV	1179469	1506123	26.26%	3.063%
23	15.271	1164	1171	1174	rBV4	28986	107271	1.87%	0.218%
24	15.340	1174	1177	1182	rVB	968914	1225445	21.36%	2.493%
25	15.694	1201	1208	1214	rBV3	31388	161257	2.81%	0.328%

Sum of corrected areas: 49165114

LSC Report - Integrated Chromatogram

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Operator : SJ/MA
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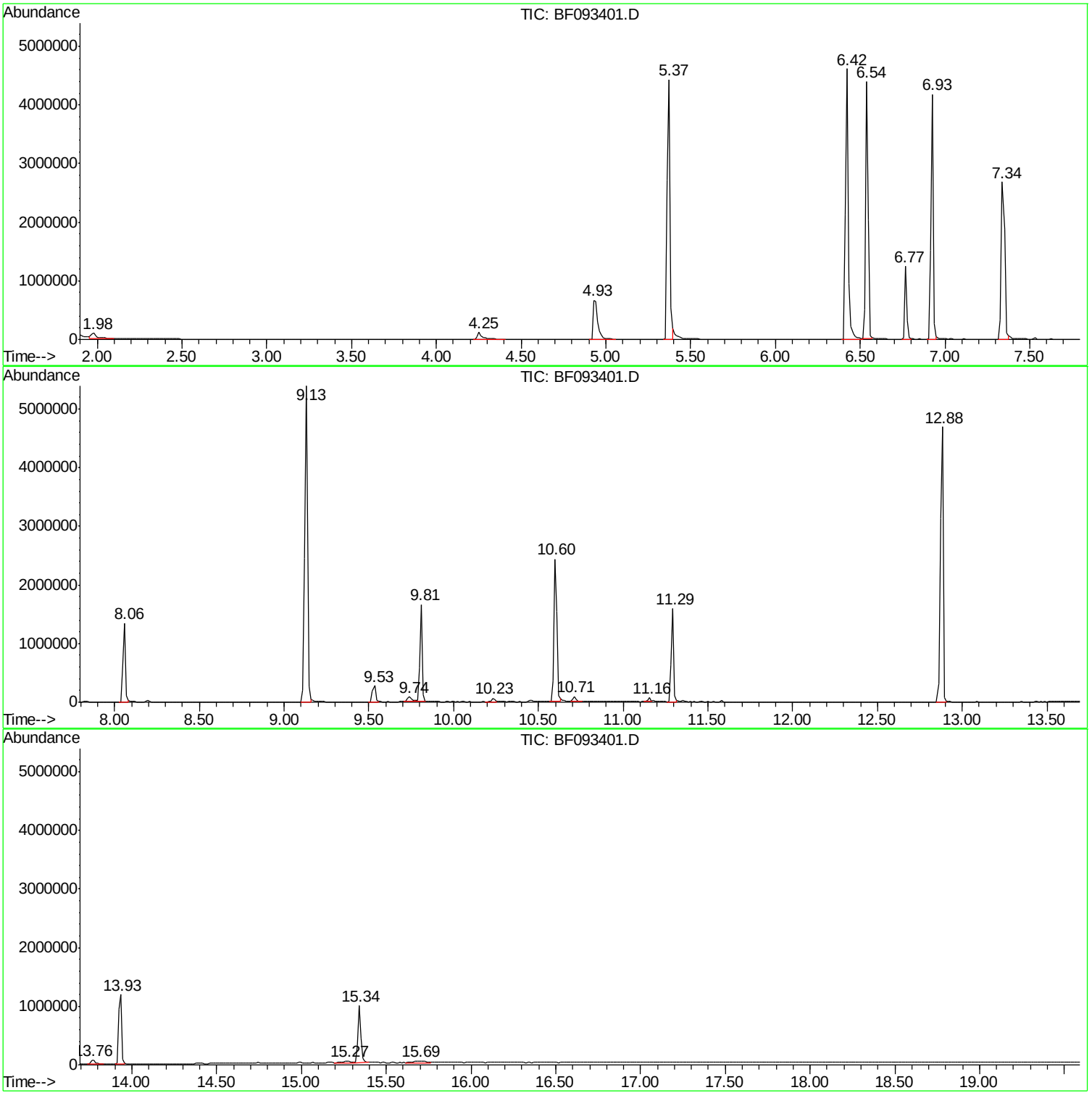
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF030617\
Data File : BF093401.D
Acq On : 6 Mar 2017 15:28
Operator : SJ/MA
Sample : I2076-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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

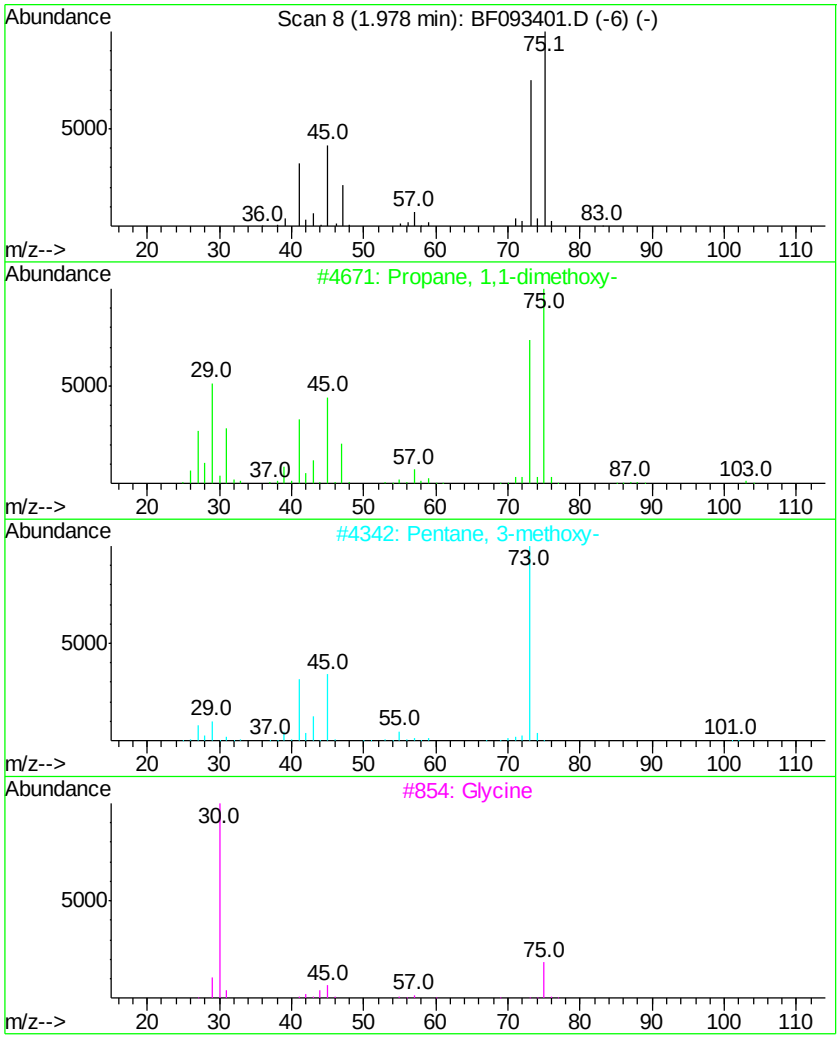
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

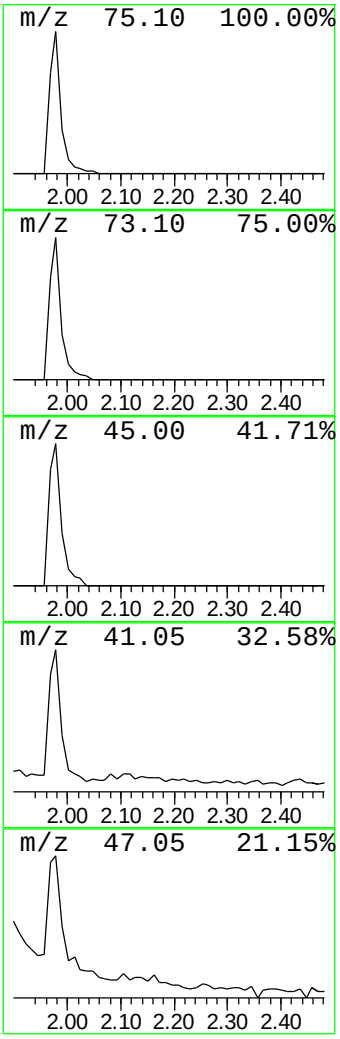
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.98	3.23 ng	180511	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
3	Glycine	75	C2H5NO2	000056-40-6	9
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





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Acq On : 6 Mar 2017 15:28
Operator : SJ/MA
Sample : I2076-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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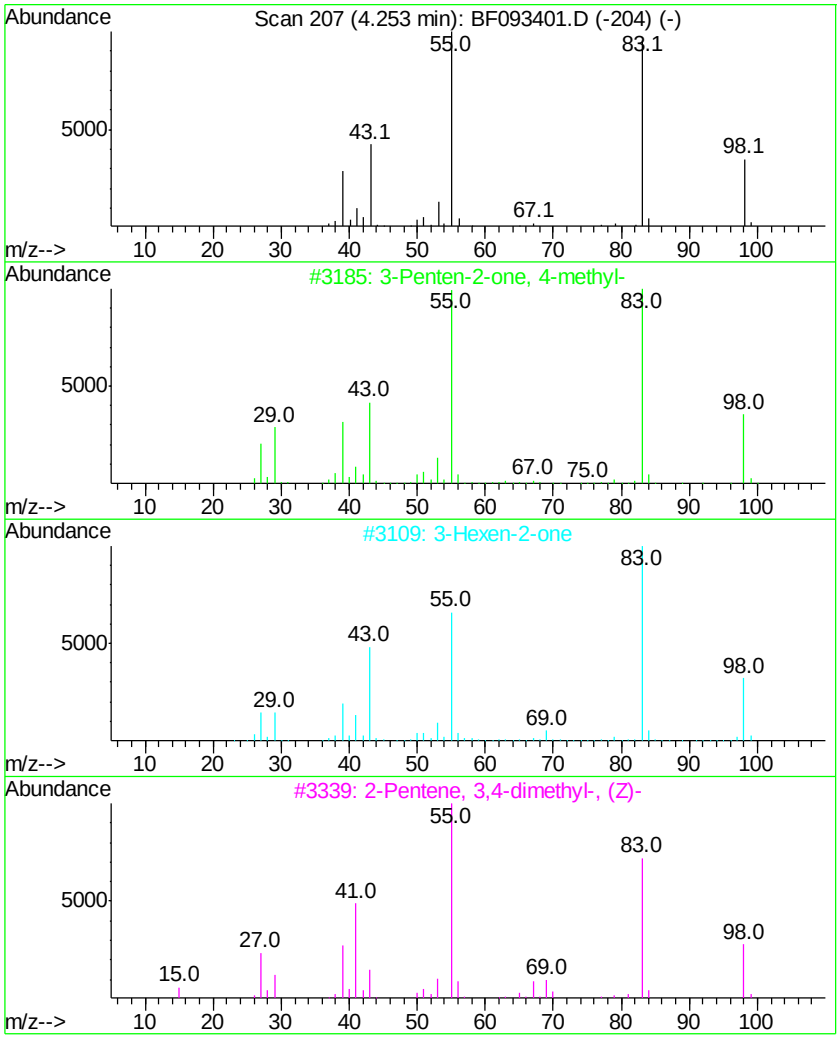
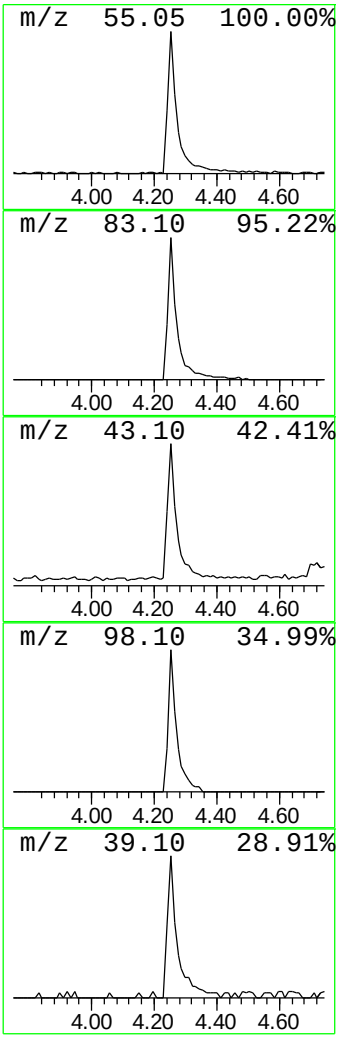
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	4.42 ng	246898	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\HPCHEM1\BNA F\Data\BF030617\
Data File : BF093401.D
Acq On : 6 Mar 2017 15:28
Operator : SJ/MA
Sample : I2076-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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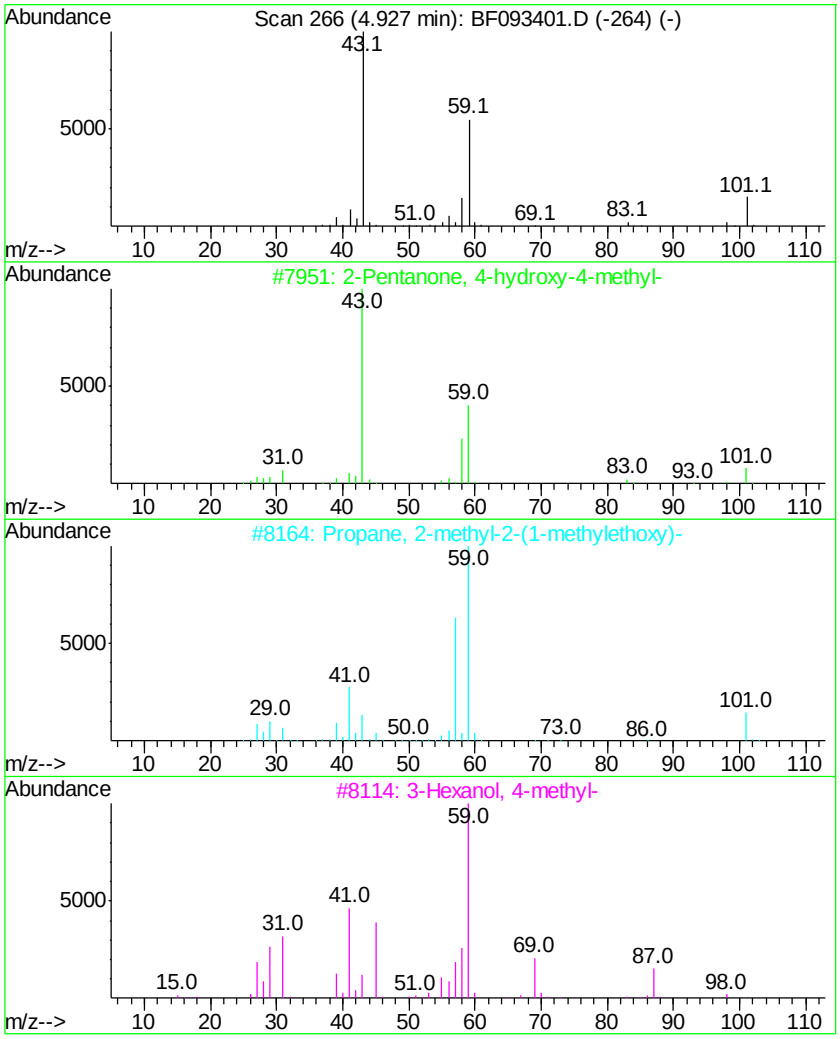
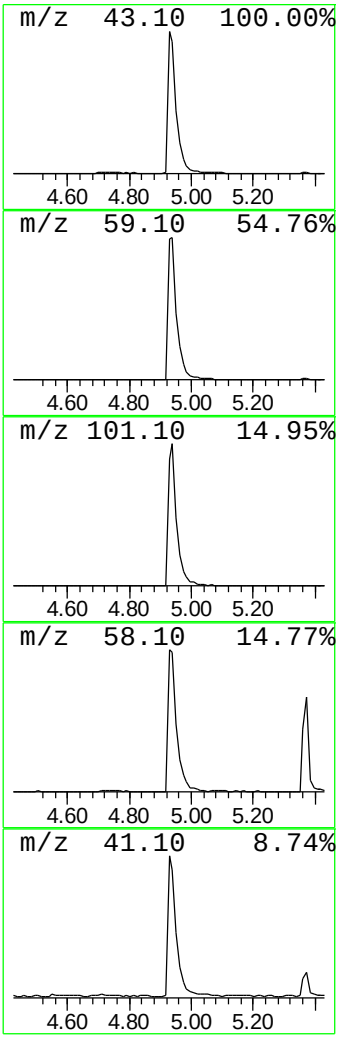
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	23.66 ng	1320630	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Operator : SJ/MA
Sample : I2076-02
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Instrument : BNA_F
ClientSampleId : 39A-7-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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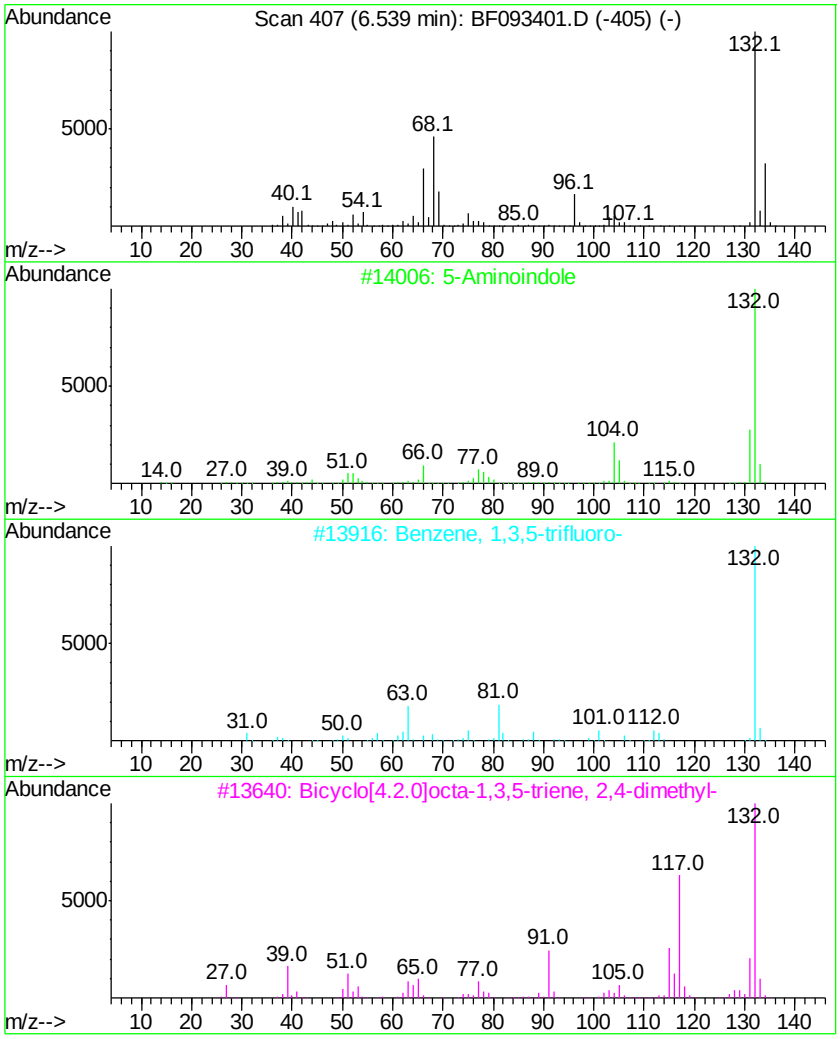
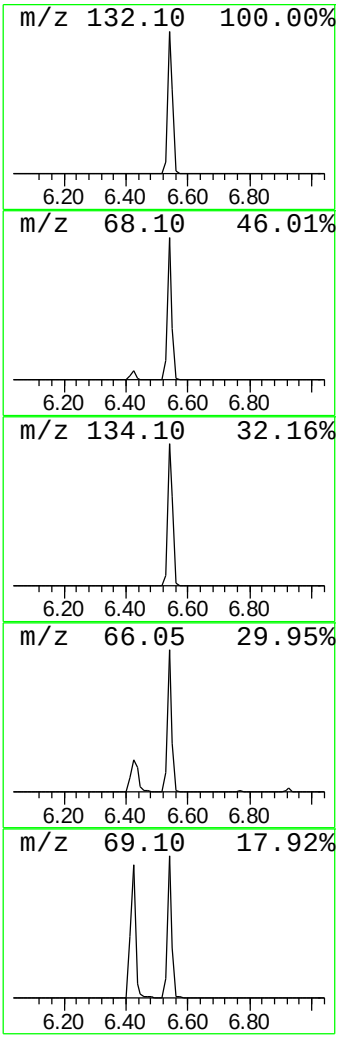
Peak Number 4 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	85.34 ng	4763110	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Operator : SJ/MA
Sample : I2076-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39A-7-9

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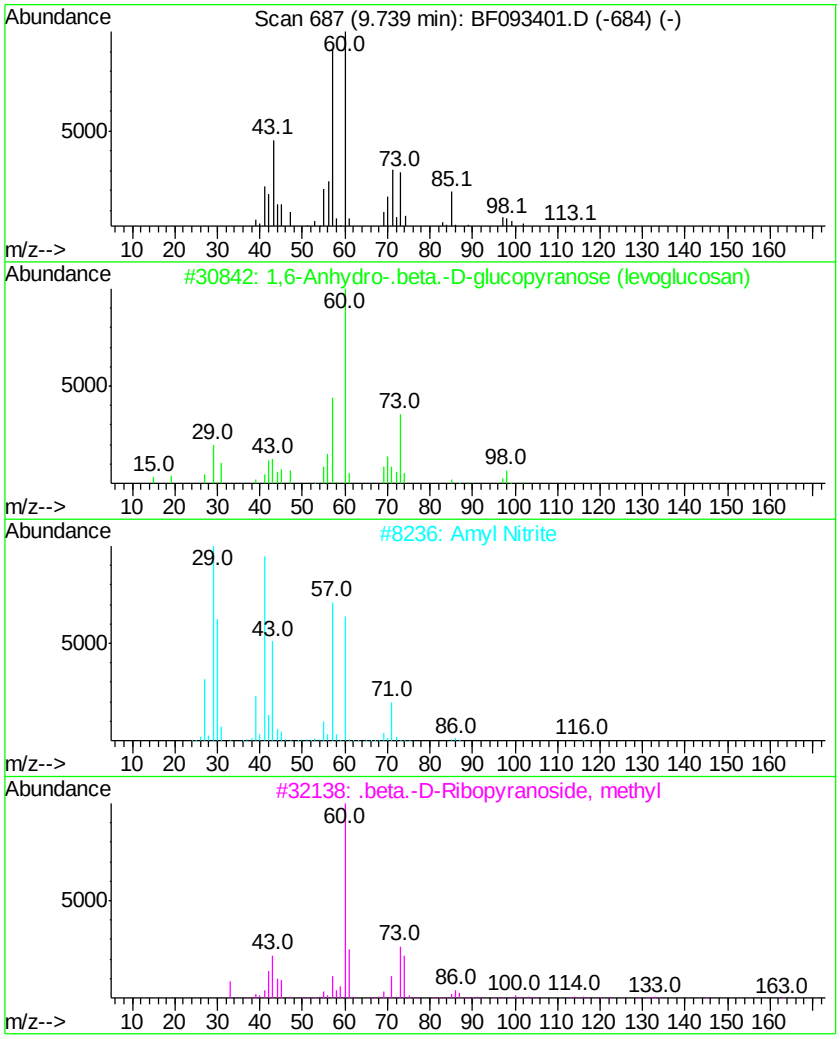
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

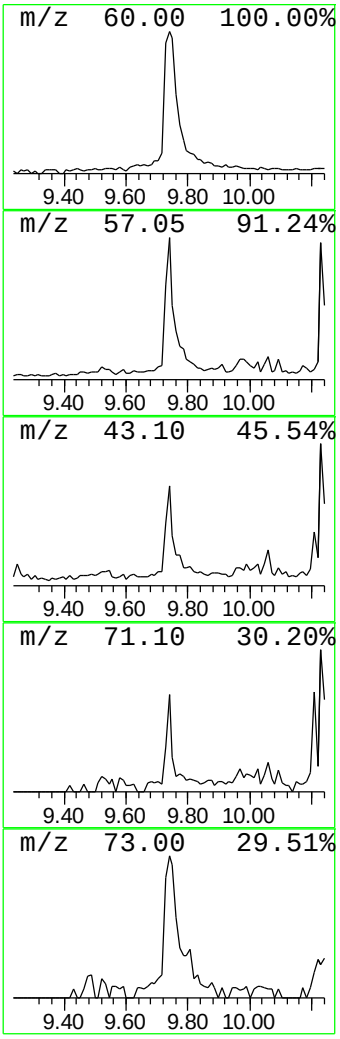
****

Peak Number 6 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	2.06 ng	164670	Acenaphthene-d10	9.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	50
2	Amyl Nitrite	117	C5H11NO2	000110-46-3	38
3	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	37
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	25
5	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	22





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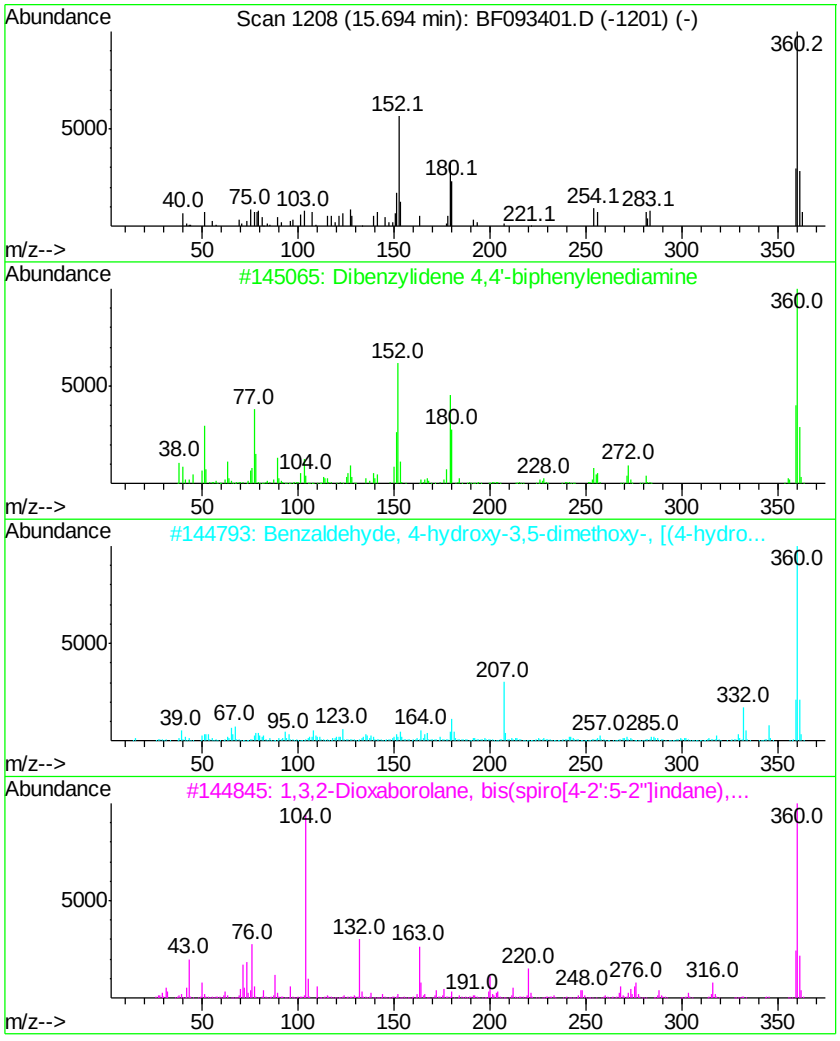
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

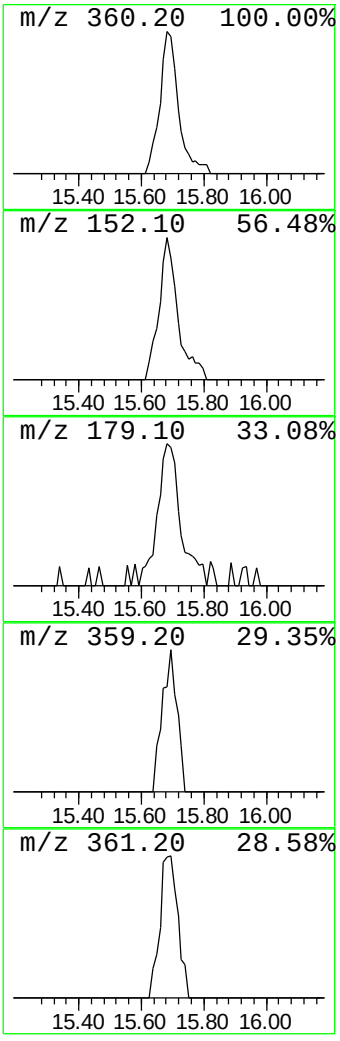
****

Peak Number 7 Dibenzylidene 4,4'-biphenyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.63 ng	161257	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	91
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43
4	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38
5	Benzoic acid, 4-(3,4-dihydro-2,4...	361	C20H15N3O4	317326-96-8	35





Tentatively Identified Compound (LSC) summary

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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...	1.98	3.2	ng	180511	1	6.77	1116290	20.0
3-Penten-2-one, 4...	4.25	4.4	ng	246898	1	6.77	1116290	20.0
2-Pentanone, 4-hy...	4.93	23.7	ng	1320630	1	6.77	1116290	20.0
unknown6.54	6.54	85.3	ng	4763110	1	6.77	1116290	20.0
1,6-Anhydro-.beta...	9.74	2.1	ng	164670	3	9.81	1600870	20.0
Dibenzylidene 4,4...	15.69	2.6	ng	161257	6	15.34	1225450	20.0