LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088655.D
Acq On : 3 Jul 2016 18:57
Operator : UM/SJ
Sample : H3822-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

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-BF063016.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	1.633	3	4	7	rVB	4044894	5479269	100.00%	15.645%
2	1.735	7	13	17	rVB2	235070	725922	13.25%	2.073%
3	2.021	36	38	41	rBV	64147	74501	1.36%	0.213%
4	4.959	292	295	300	rBB	161826	238306	4.35%	0.680%
5	5.381	329	332	334	rBV	2564574	2760780	50.39%	7.883%
6	6.422	419	423	425	rBV	2606214	2971870	54.24%	8.486%
7	6.547	431	434	437	rBV	2205073	3091530	56.42%	8.827%
8	6.787	452	455	457	rBV	527493	634211	11.57%	1.811%
9	6.936	466	468	471	rVB	1945945	2336914	42.65%	6.673%
10	7.347	501	504	506	rBV	1843578	1939957	35.41%	5.539%
11	8.067	564	567	569	rBV	1058148	917540	16.75%	2.620%
12	9.142	658	661	664	rBB	2610598	3532382	64.47%	10.086%
13	9.542	693	696	698	rBV	372391	428734	7.82%	1.224%
14	9.816	717	720	722	rBV	1161177	1013966	18.51%	2.895%
15	10.605	786	789	791	rBV	2130612	2271803	41.46%	6.487%
16	10.731	798	800	804	rVB	83740	86252	1.57%	0.246%
17	11.291	847	849	852	rBV	1124142	1023311	18.68%	2.922%
18	12.879	985	988	991	rBV	2920915	3230220	58.95%	9.223%
19	13.851	1070	1073	1076	rBV	61818	175273	3.20%	0.500%
20	13.919	1076	1079	1081	rVB	969702	1007918	18.40%	2.878%
21	14.560	1133	1135	1137	rVB	406652	353809	6.46%	1.010%
22	15.302	1197	1200	1203	rBV	476636	727636	13.28%	2.078%

Sum of corrected areas: 35022104

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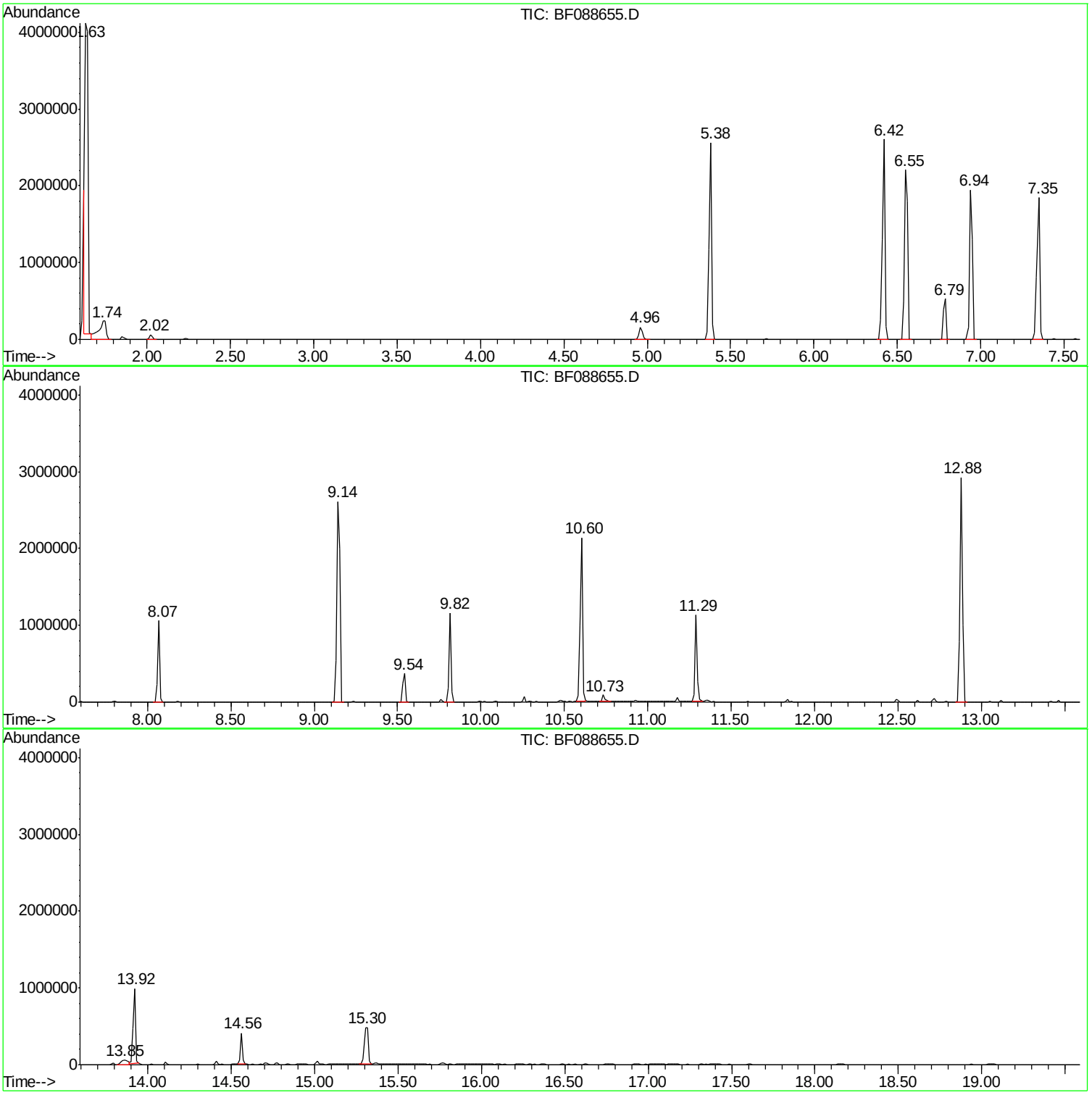
Instrument :
BNA_F
ClientSampleId :
C9-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

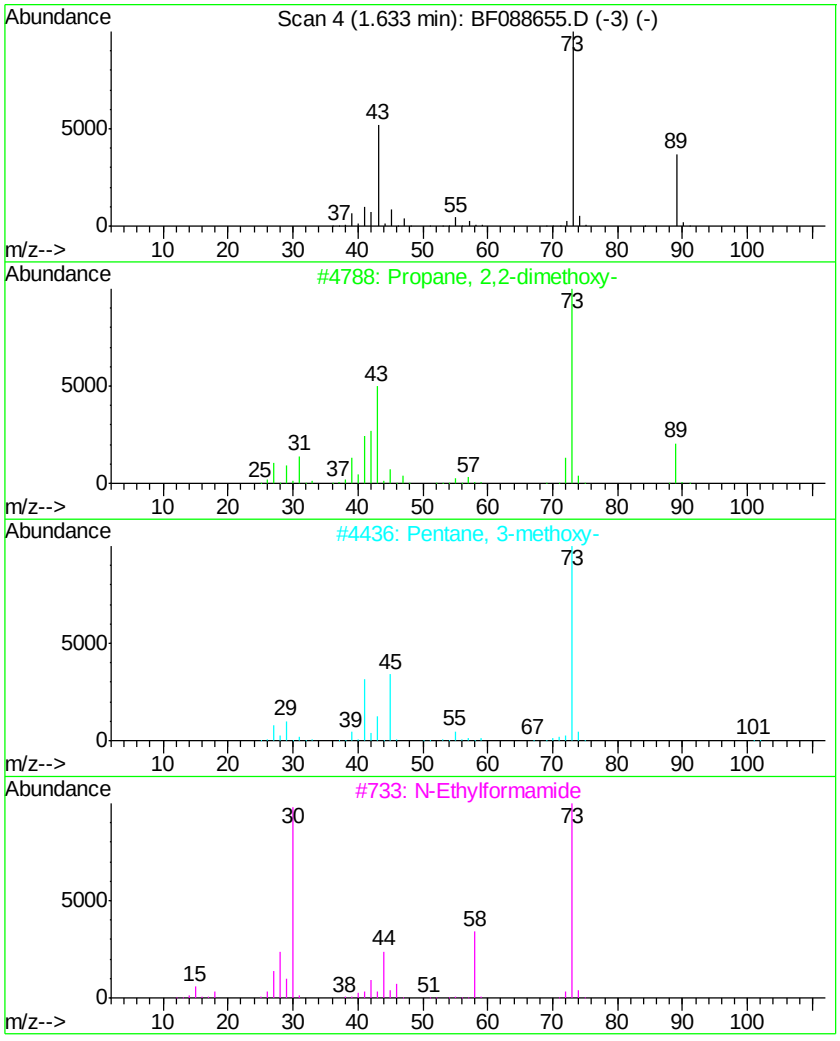
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

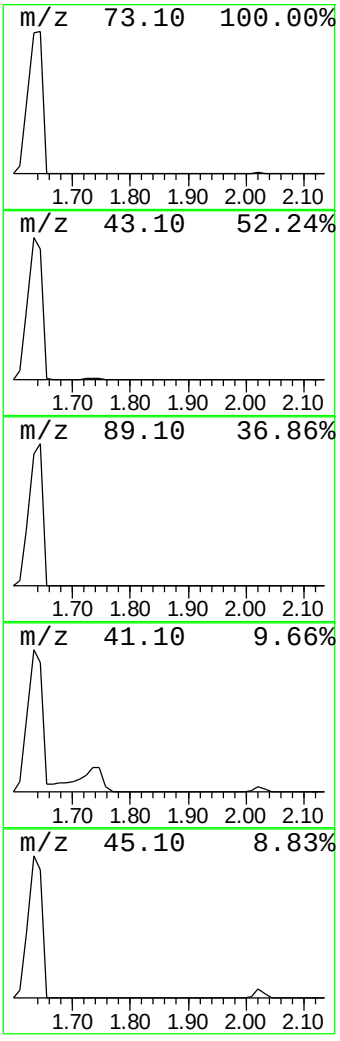
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.63	172.79 ng	5479270	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088655.D
Acq On : 3 Jul 2016 18:57
Operator : UM/SJ
Sample : H3822-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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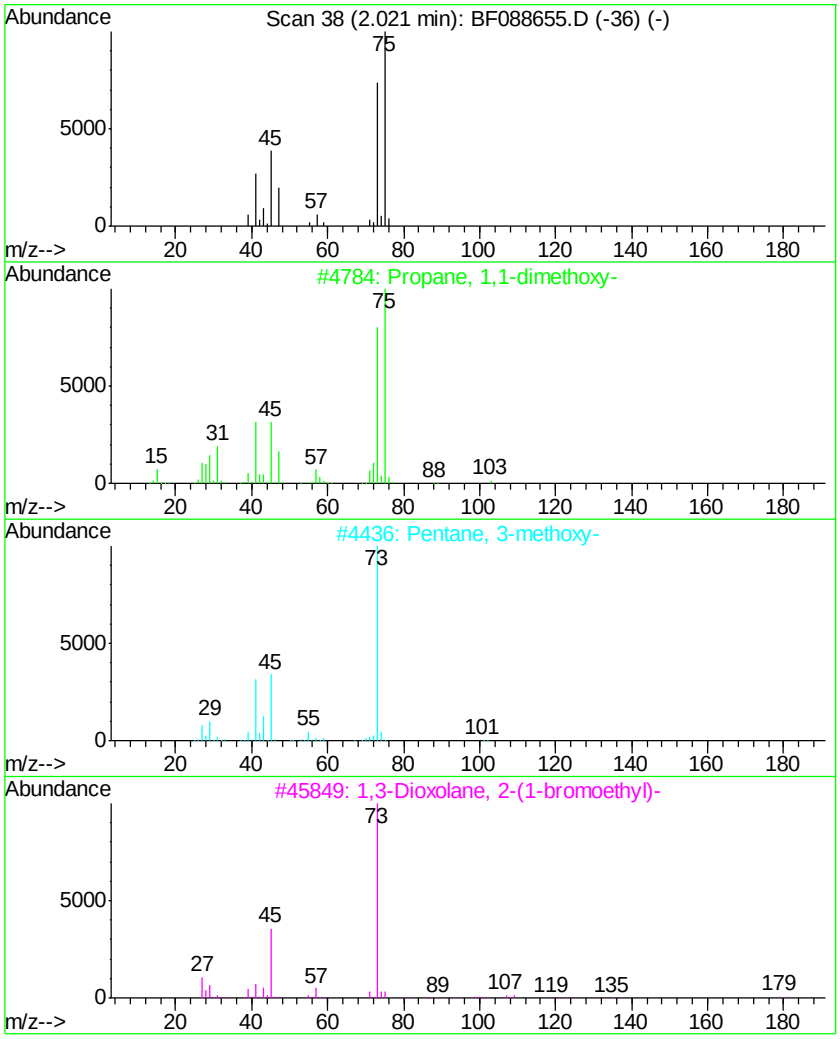
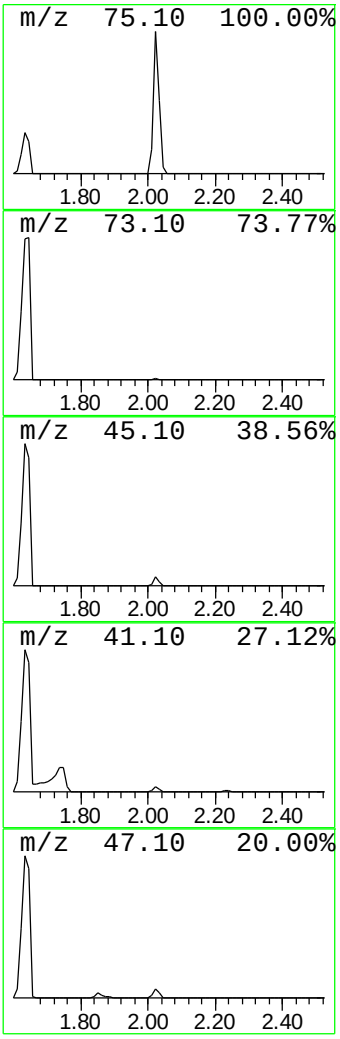
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.35 ng	74501	1,4-Dichlorobenzene-d4	6.79

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	27
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9





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Operator : UM/SJ
Sample : H3822-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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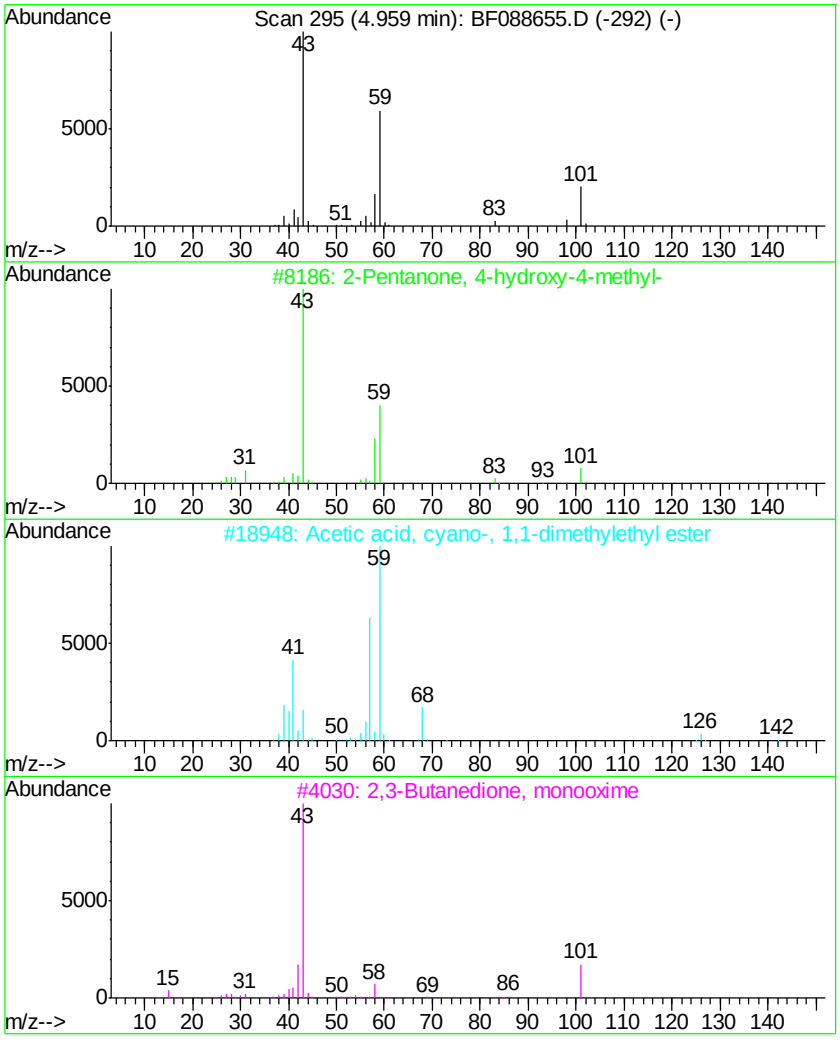
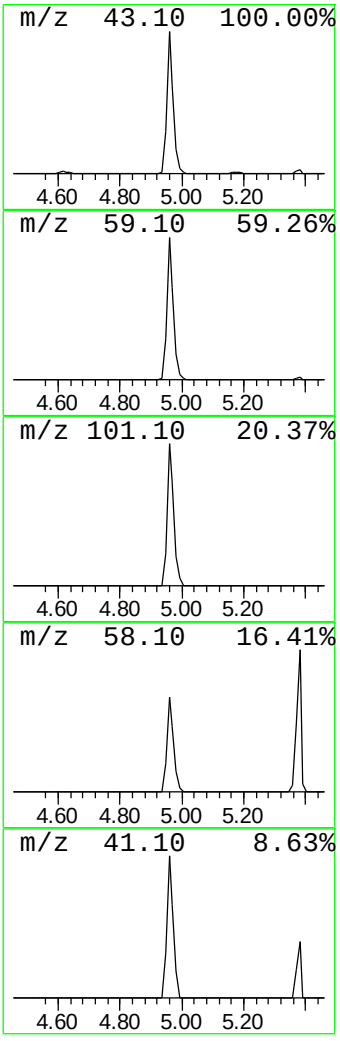
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.52 ng	238306	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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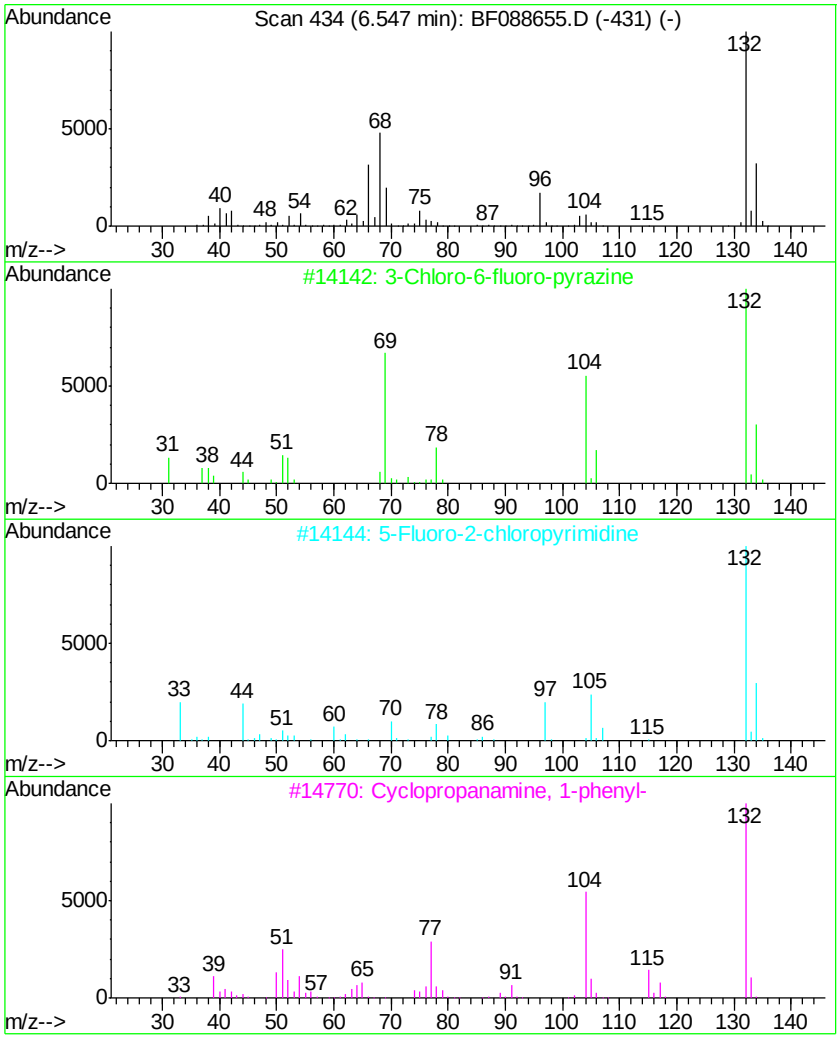
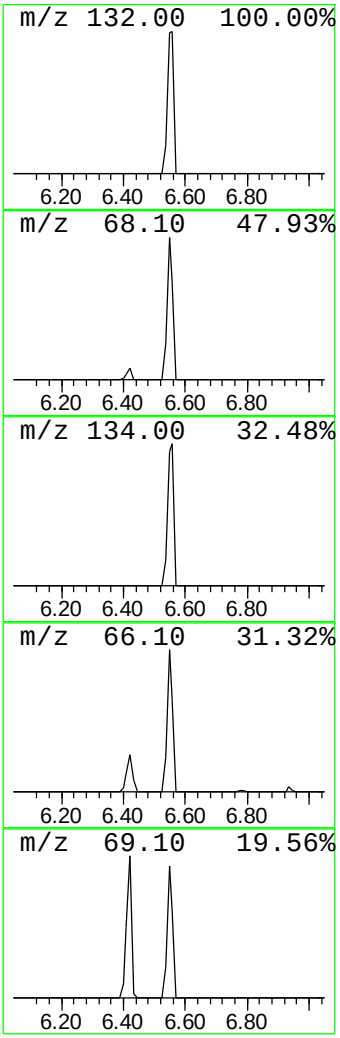
Peak Number 5 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	97.49 ng	3091530	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





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Sample : H3822-11
Misc :
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Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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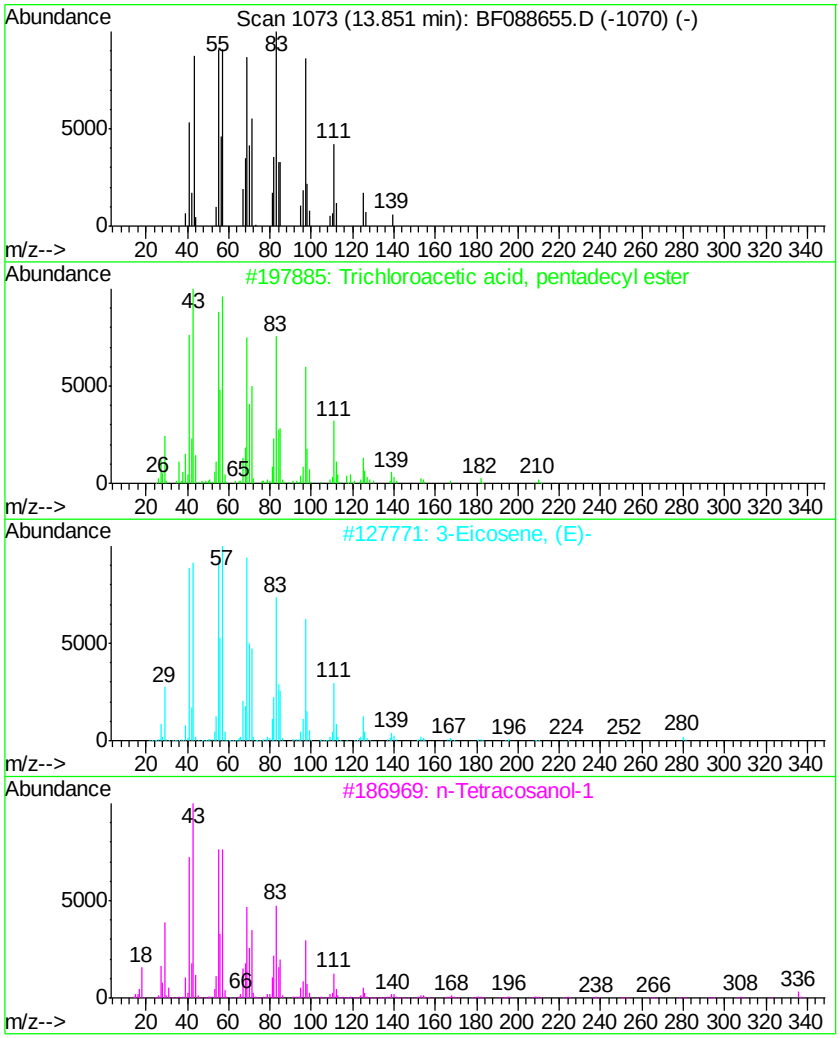
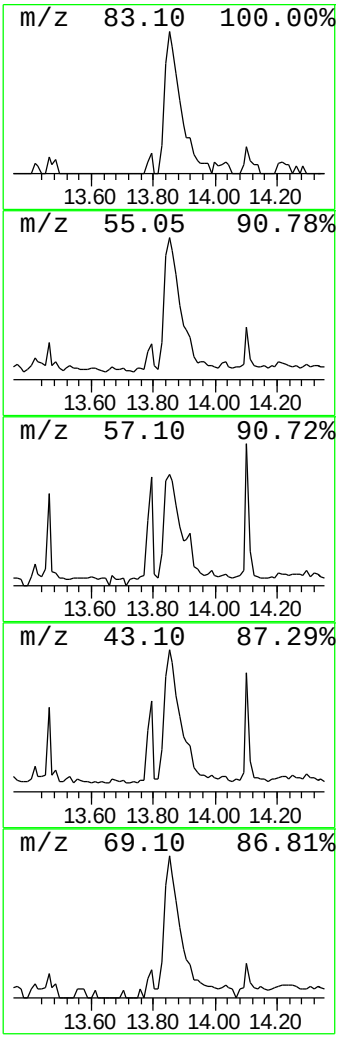
Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.48 ng	175273	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	86
5	1-Docosene	308	C22H44	001599-67-3	81





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Sample : H3822-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C9-B1(0-11)C

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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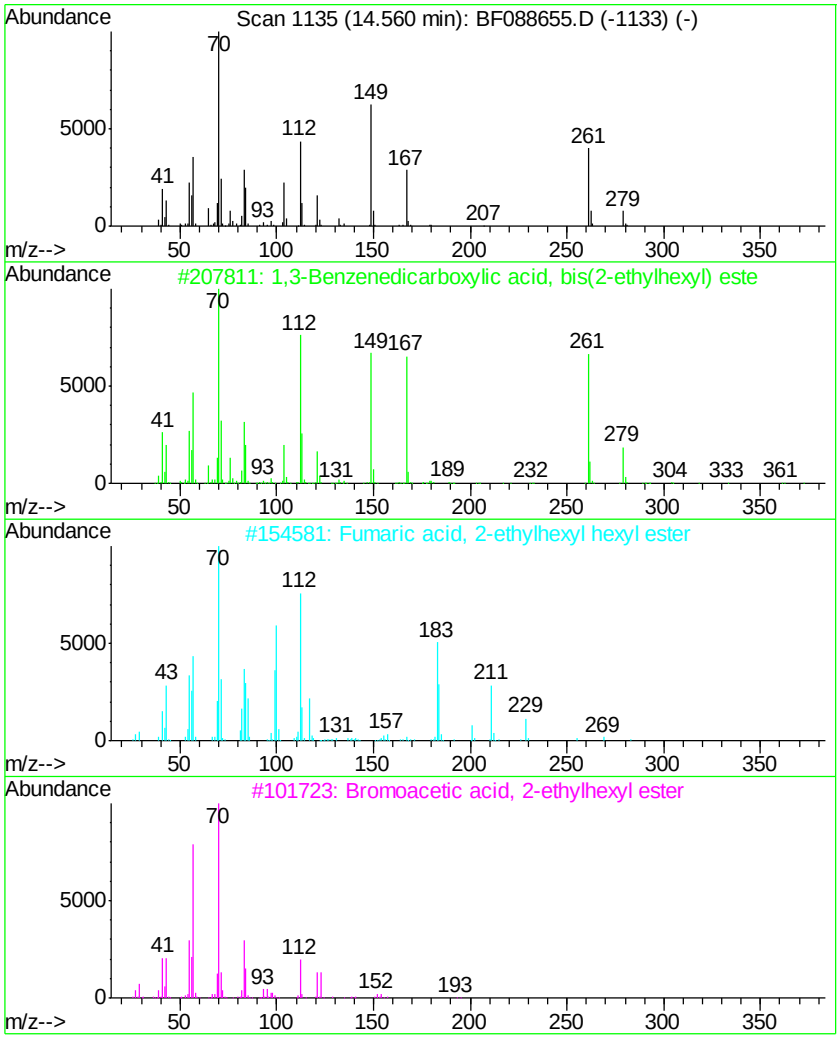
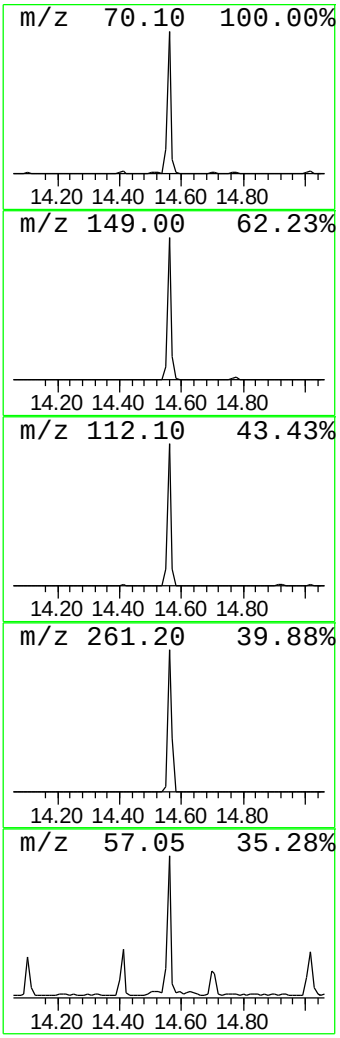
Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	7.02 ng	353809	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2	Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	22
3	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	16
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	14
5	Diisooctyl phthalate	390	C24H38O4	000131-20-4	14





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	1.63	172.8	ng	5479270	1	6.79	634211	20.0
Propane, 1,1-dime...	2.02	2.4	ng	74501	1	6.79	634211	20.0
2-Pentanone, 4-hy...	4.96	7.5	ng	238306	1	6.79	634211	20.0
unknown6.55	6.55	97.5	ng	3091530	1	6.79	634211	20.0
Trichloroacetic a...	13.85	3.5	ng	175273	5	13.92	1007920	20.0
1,3-Benzenedicarb...	14.56	7.0	ng	353809	5	13.92	1007920	20.0