LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089118.D
Acq On : 19 Jul 2016 15:12
Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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	1.735	12	13	43	rVB	1234261	2295235	100.00%	22.891%
2	2.101	43	45	57	rVB	21711	47216	2.06%	0.471%
3	3.759	189	190	199	rBV2	19630	35405	1.54%	0.353%
4	4.021	209	213	216	rBV	567655	909862	39.64%	9.074%
5	4.536	256	258	260	rVB	45976	62030	2.70%	0.619%
6	4.764	273	278	280	rBV	534090	887979	38.69%	8.856%
7	5.210	315	317	319	rBV	115959	139355	6.07%	1.390%
8	5.610	350	352	355	rBB	183892	162323	7.07%	1.619%
9	6.273	408	410	412	rBV	76918	95451	4.16%	0.952%
10	6.387	418	420	422	rBV	322783	264058	11.50%	2.633%
11	6.616	438	440	443	rBB	277503	282480	12.31%	2.817%
12	6.776	452	454	456	rVB	820057	685896	29.88%	6.841%
13	7.187	487	490	492	rBV	602732	539901	23.52%	5.385%
14	7.908	550	553	555	rBV	486018	401634	17.50%	4.006%
15	8.982	645	647	650	rBV	896857	988855	43.08%	9.862%
16	9.382	680	682	684	rBB	47012	35592	1.55%	0.355%
17	9.656	703	706	708	rBV	445746	409894	17.86%	4.088%
18	10.433	772	774	777	rVB	152968	137362	5.98%	1.370%
19	11.131	832	835	837	rVV	368135	353846	15.42%	3.529%
20	11.714	884	886	887	rVB	26834	36235	1.58%	0.361%
21	12.708	971	973	975	rBV	648441	544883	23.74%	5.434%
22	13.634	1049	1054	1058	rBV2	22962	44522	1.94%	0.444%
23	13.748	1061	1064	1066	rBV	354294	334969	14.59%	3.341%
24	14.925	1165	1167	1172	rVB3	12397	23019	1.00%	0.230%
25	15.097	1180	1182	1185	rBV	203590	242731	10.58%	2.421%
26	15.634	1227	1229	1233	rBV3	10422	26520	1.16%	0.264%
27	16.068	1264	1267	1272	rVB4	14228	39656	1.73%	0.395%

Sum of corrected areas: 10026909

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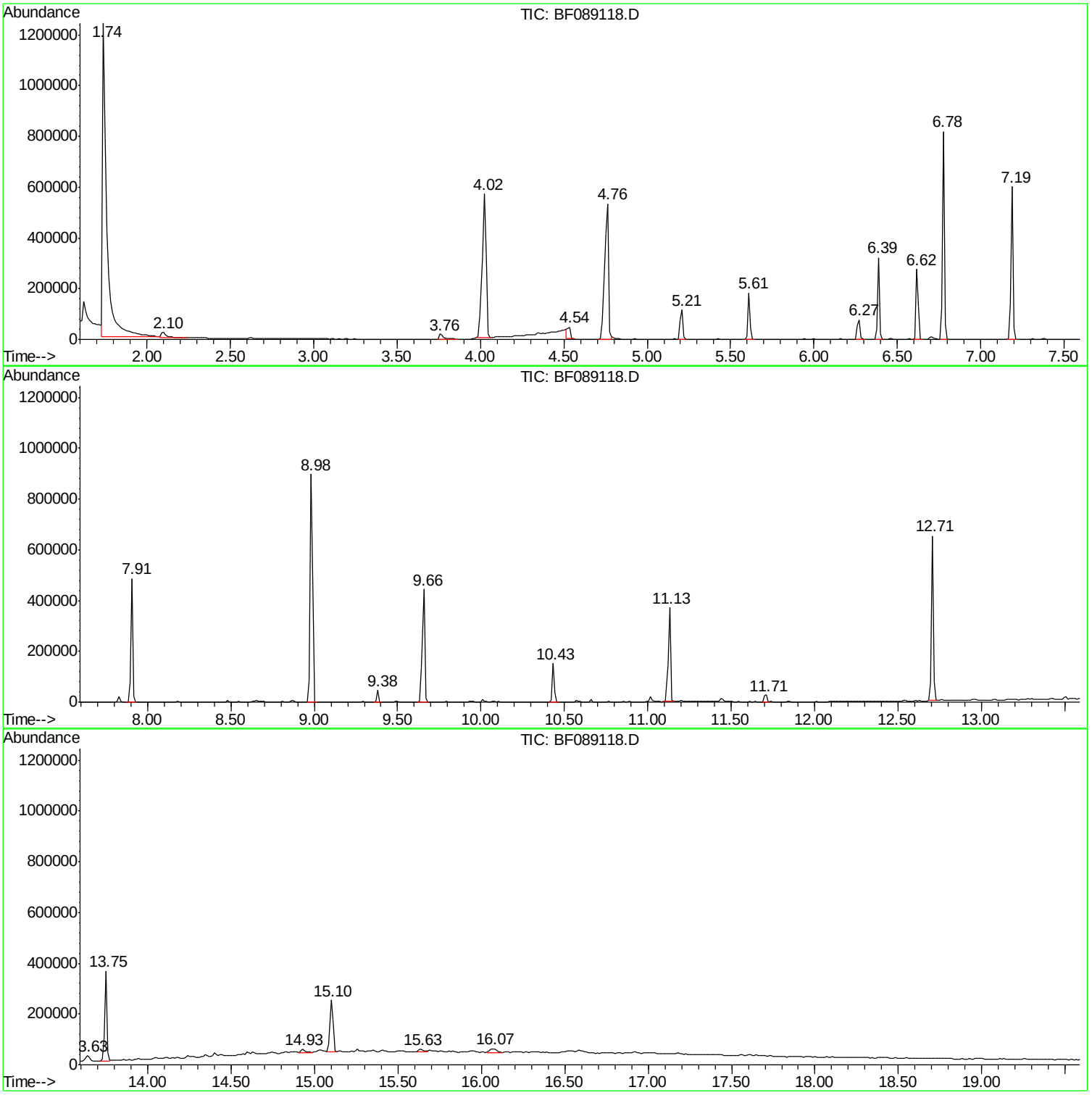
ClientSampleId : PO-001

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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Data File : BF089118.D
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Operator : UM/SJ
Sample : H4071-01
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TIC Library : C:\Database\NIST11.L
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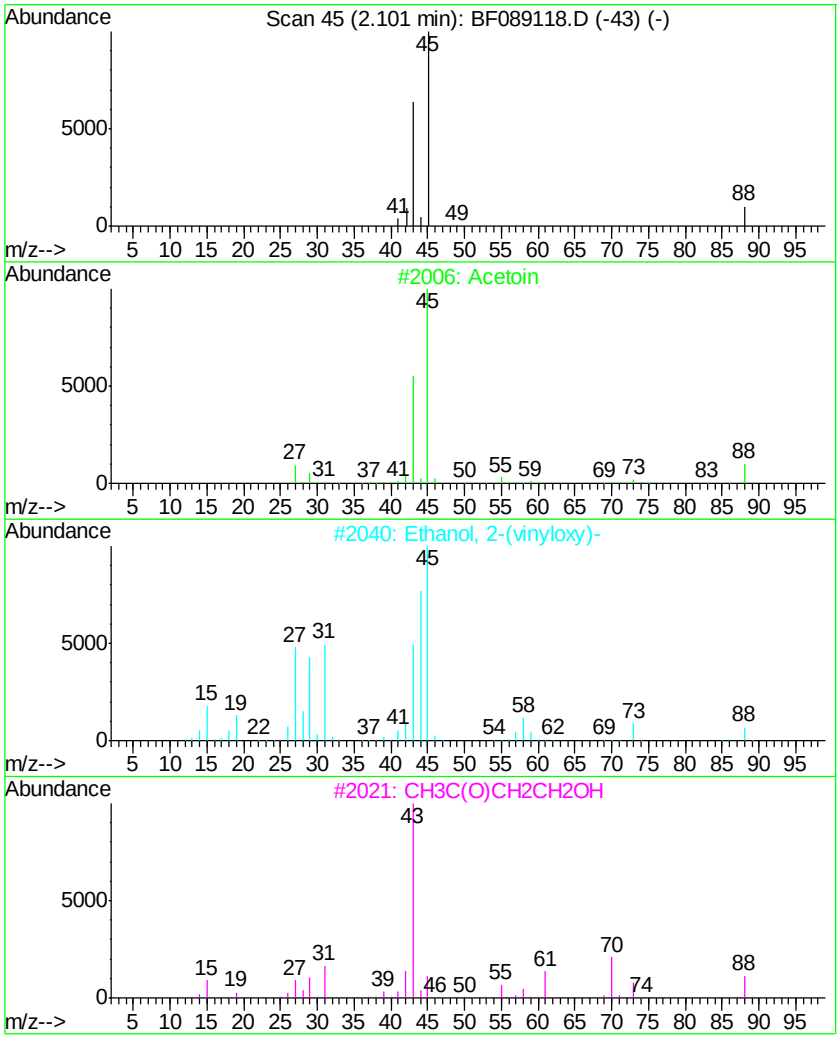
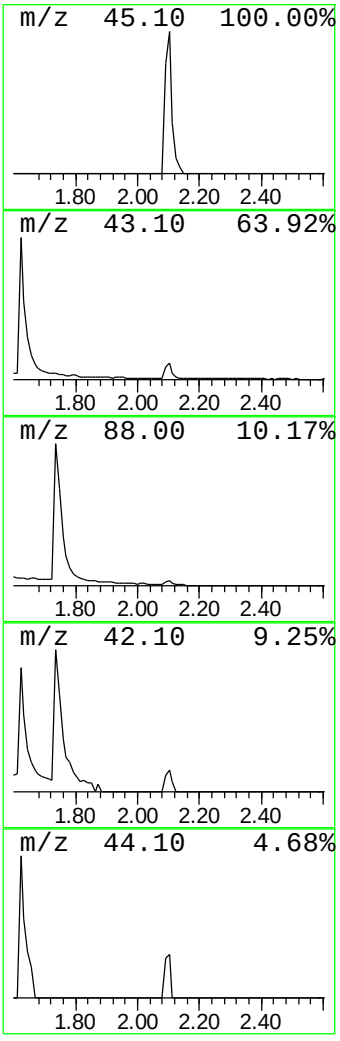
Peak Number 2 unknown2.10 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	3.34 ng	47216	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetoin	88	C4H8O2	000513-86-0	9
2	Ethanol, 2-(vinyloxy)-	88	C4H8O2	000764-48-7	9
3	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	7
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	7
5	Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	5





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Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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

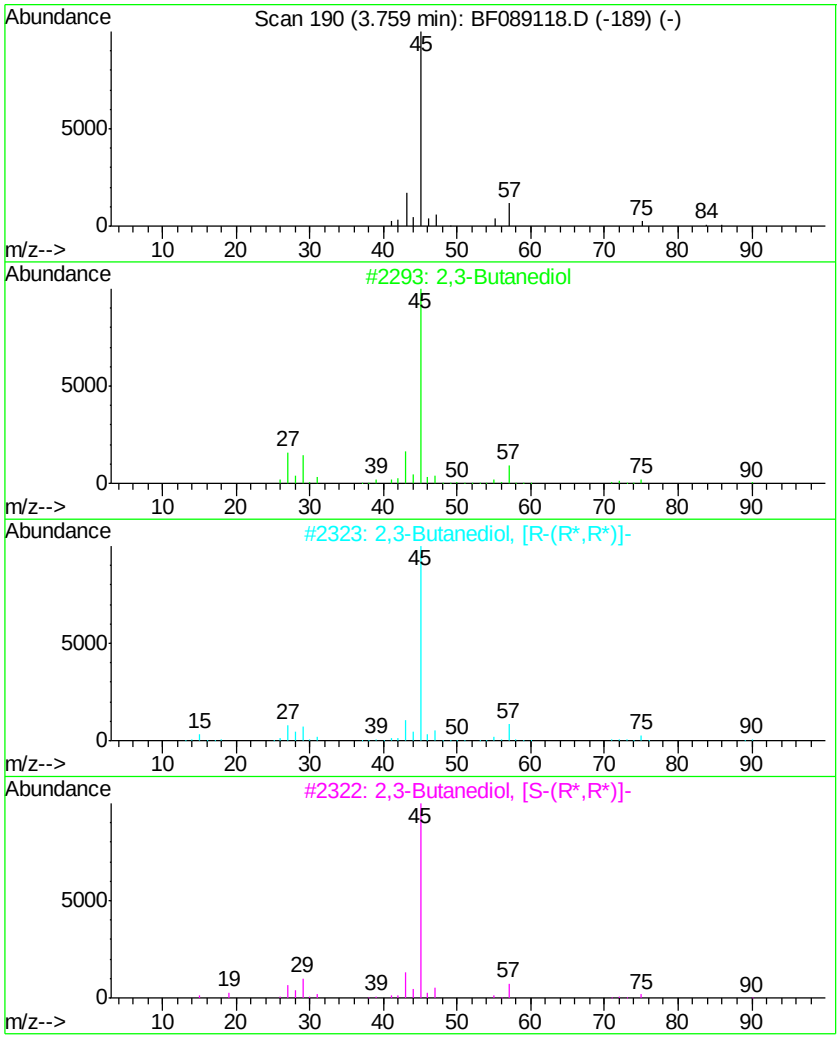
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

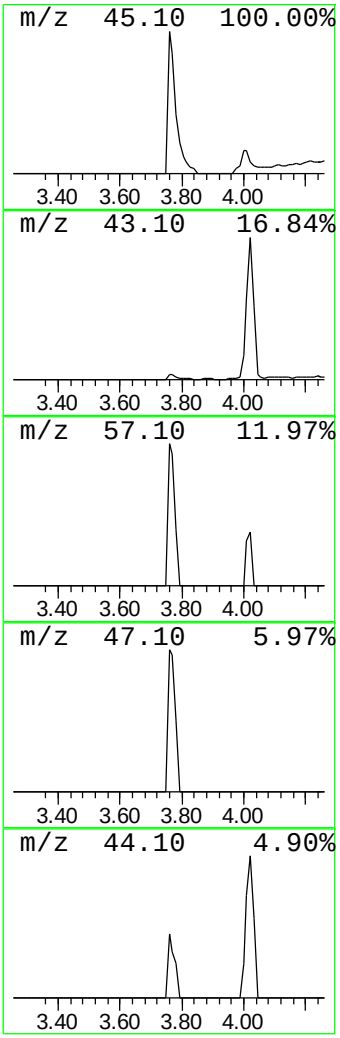
****

Peak Number 3 2,3-Butanediol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	2.51 ng	35405	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanediol	90	C4H10O2	000513-85-9	74
2	2,3-Butanediol, [R-(R*,R*)]-	90	C4H10O2	024347-58-8	74
3	2,3-Butanediol, [S-(R*,R*)]-	90	C4H10O2	019132-06-0	74
4	Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	39
5	Ethanol, 2-methoxy-, carbonate (...	178	C7H14O5	000626-84-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089118.D
Acq On : 19 Jul 2016 15:12
Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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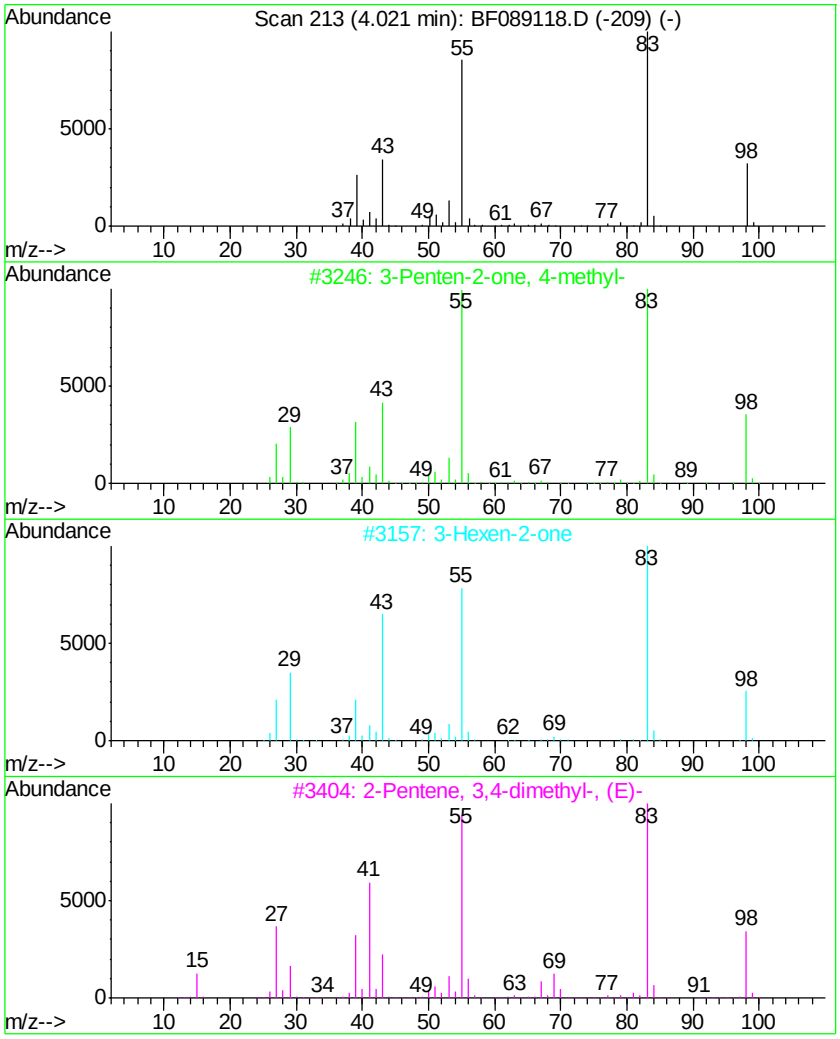
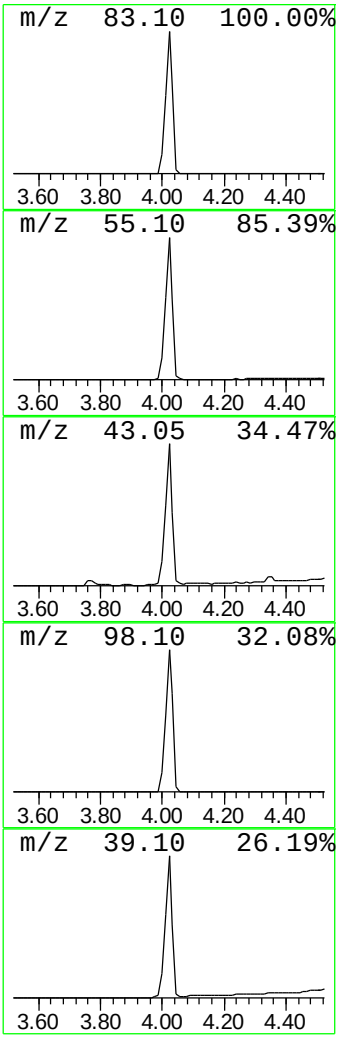
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	64.42 ng	909862	1,4-Dichlorobenzene-d4	6.62

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





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Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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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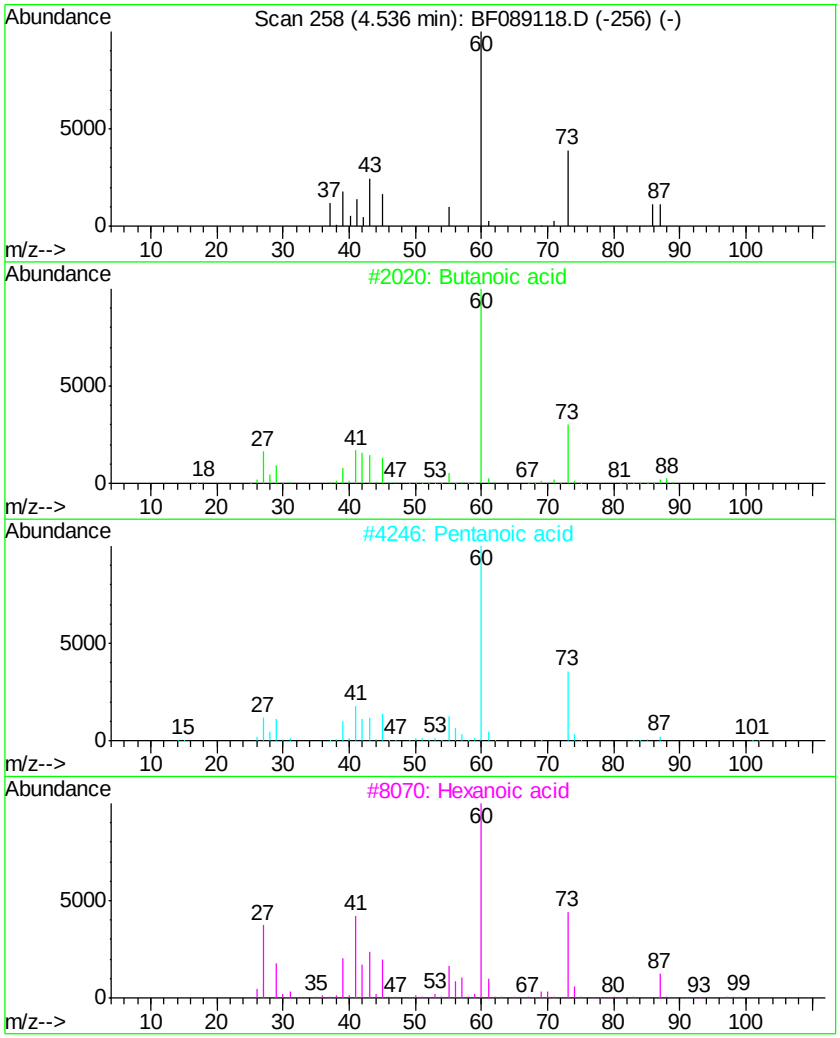
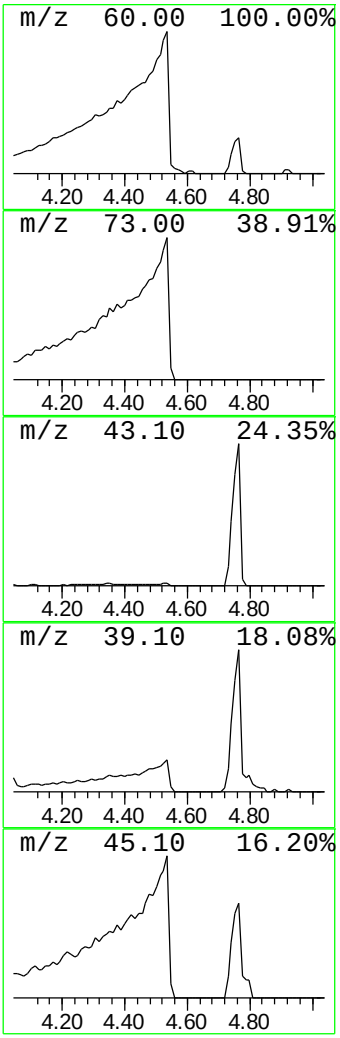
Peak Number 5 unknown4.54 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	4.39 ng	62030	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	28
2	Pentanoic acid	102	C5H10O2	000109-52-4	9
3	Hexanoic acid	116	C6H12O2	000142-62-1	9
4	.beta.-Methyl xyloside	164	C6H12O5	1000130-04-0	9
5	Urea	60	CH4N2O	000057-13-6	7





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Data File : BF089118.D
Acq On : 19 Jul 2016 15:12
Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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

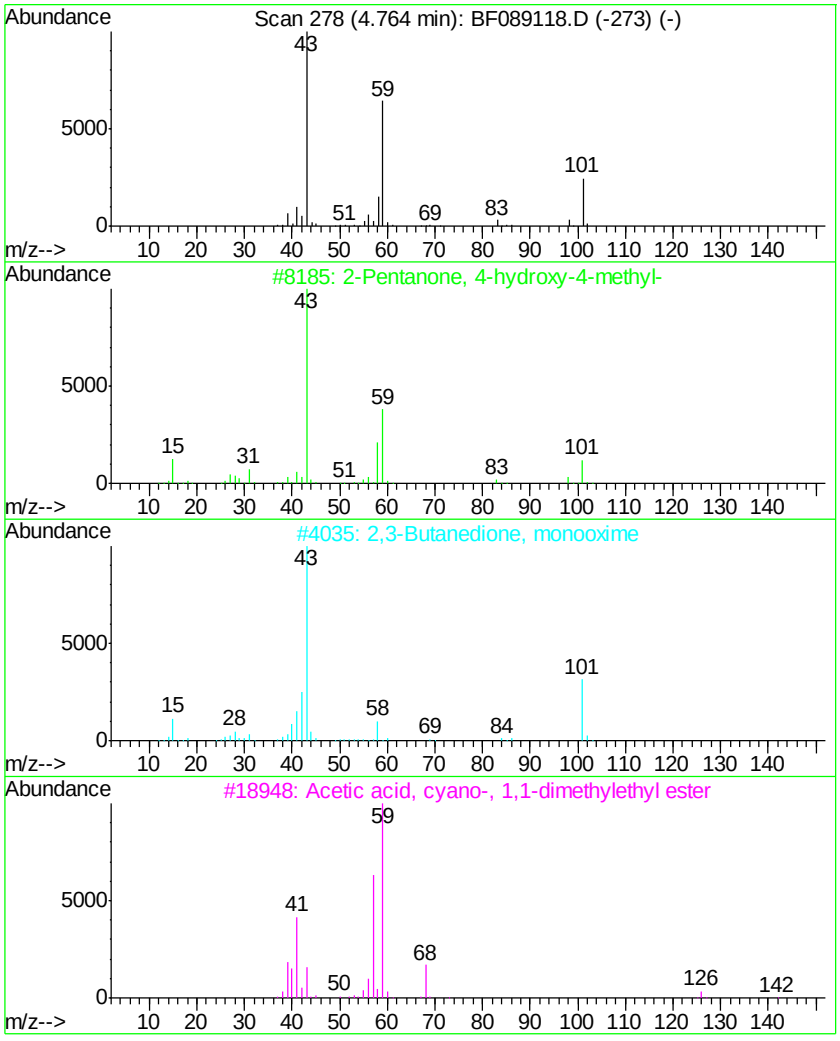
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

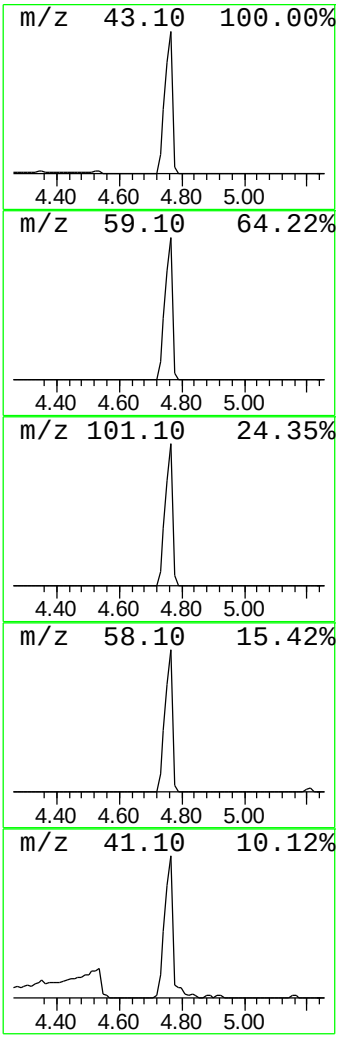
****

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	62.87 ng	887979	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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

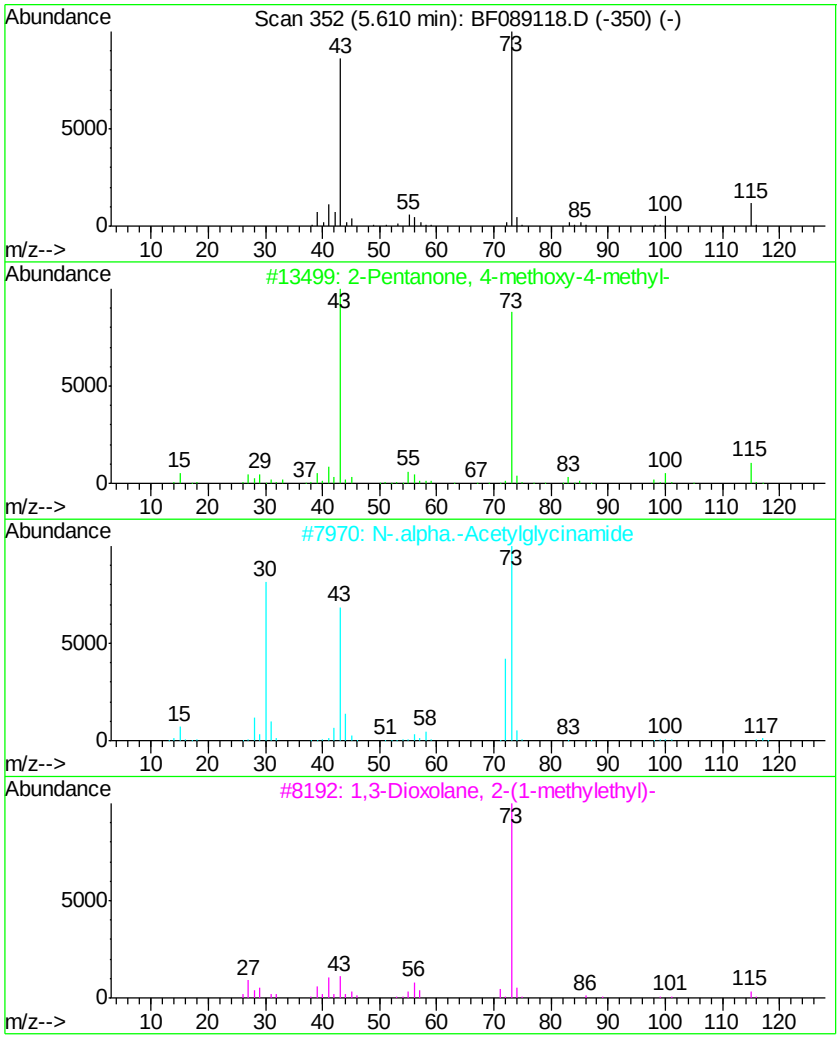
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

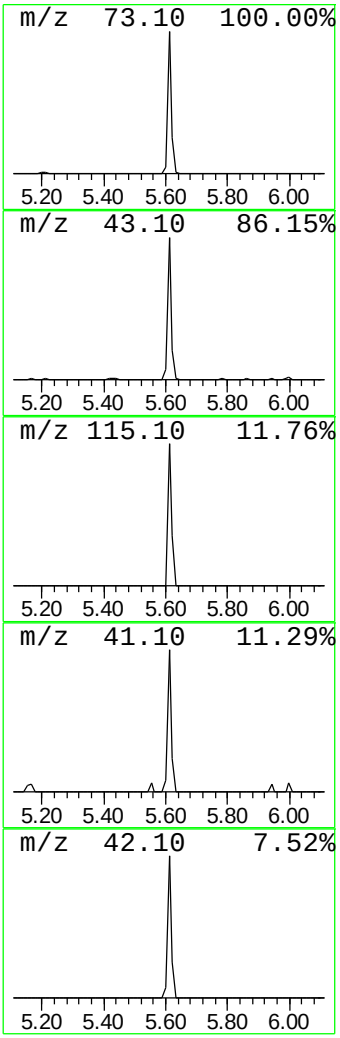
****

Peak Number 7 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	11.49 ng	162323	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9





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Instrument : BNA_F
ClientSampleId : PO-001

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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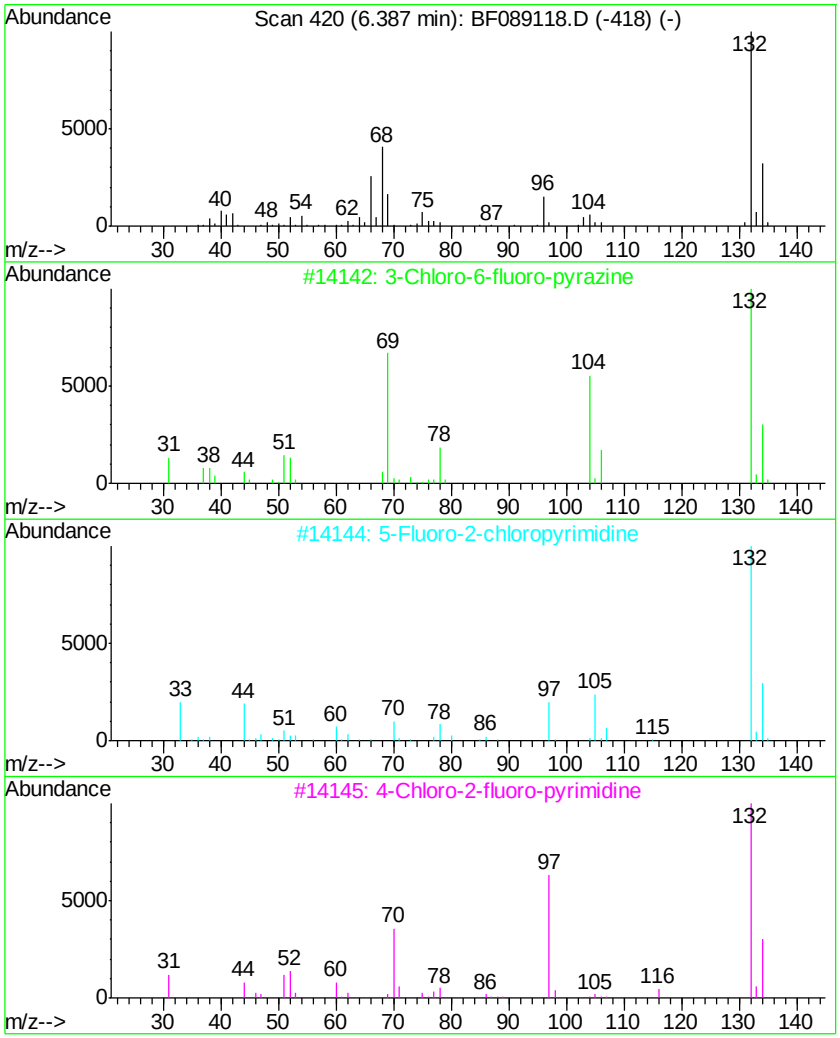
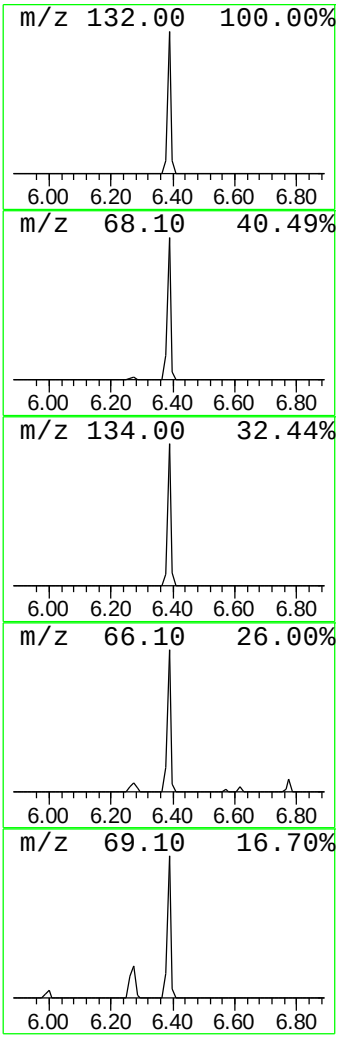
Peak Number 8 unknown6.39 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	18.70 ng	264058	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





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TIC Library : C:\Database\NIST11.L
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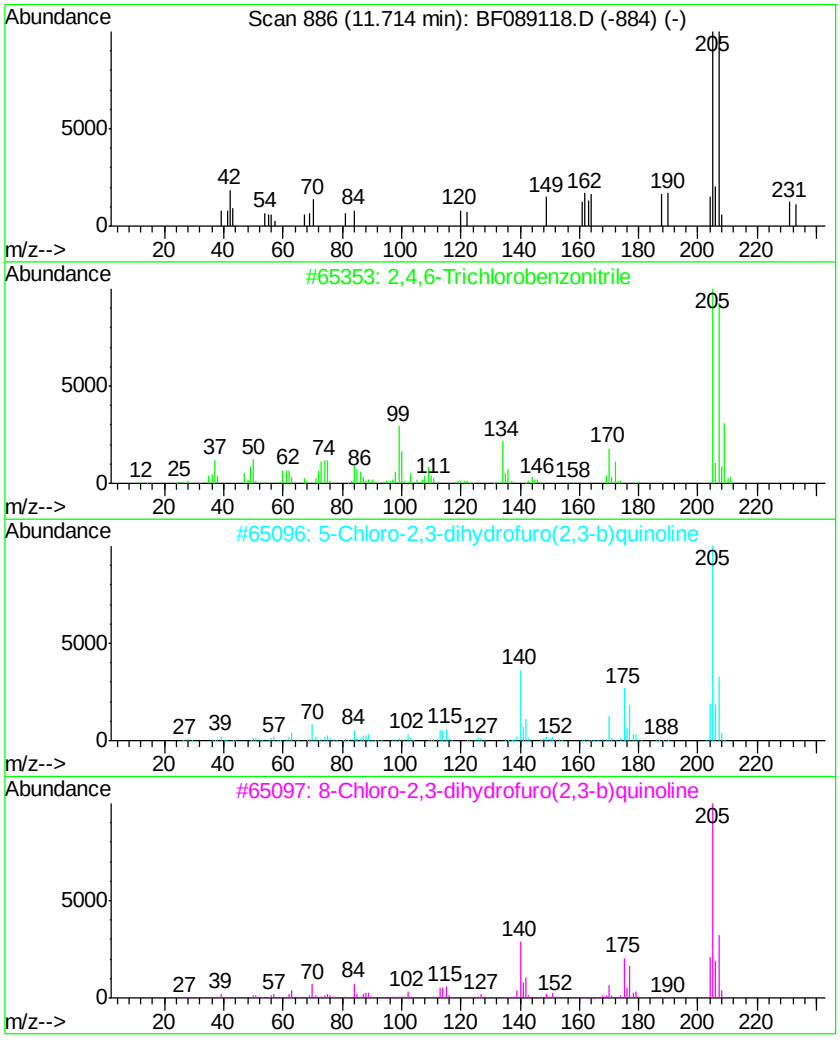
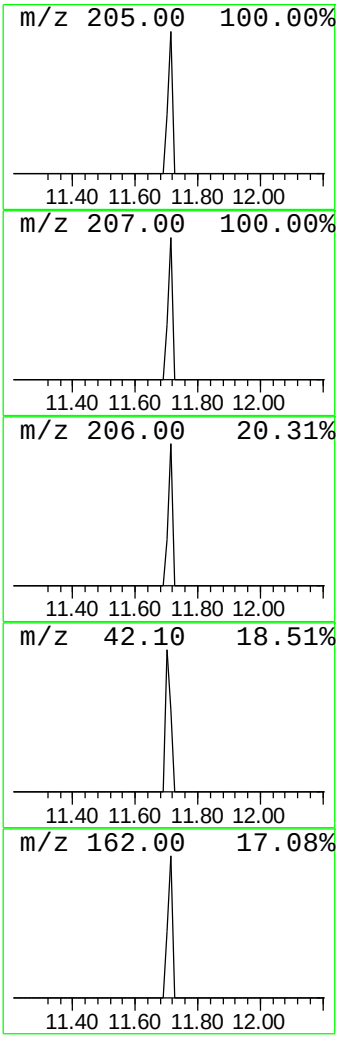
****

Peak Number 10 2,4,6-Trichlorobenzonitrile Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	2.05 ng	36235	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	53
2	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	43
3	8-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	095322-67-1	43
4	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	43
5	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	42





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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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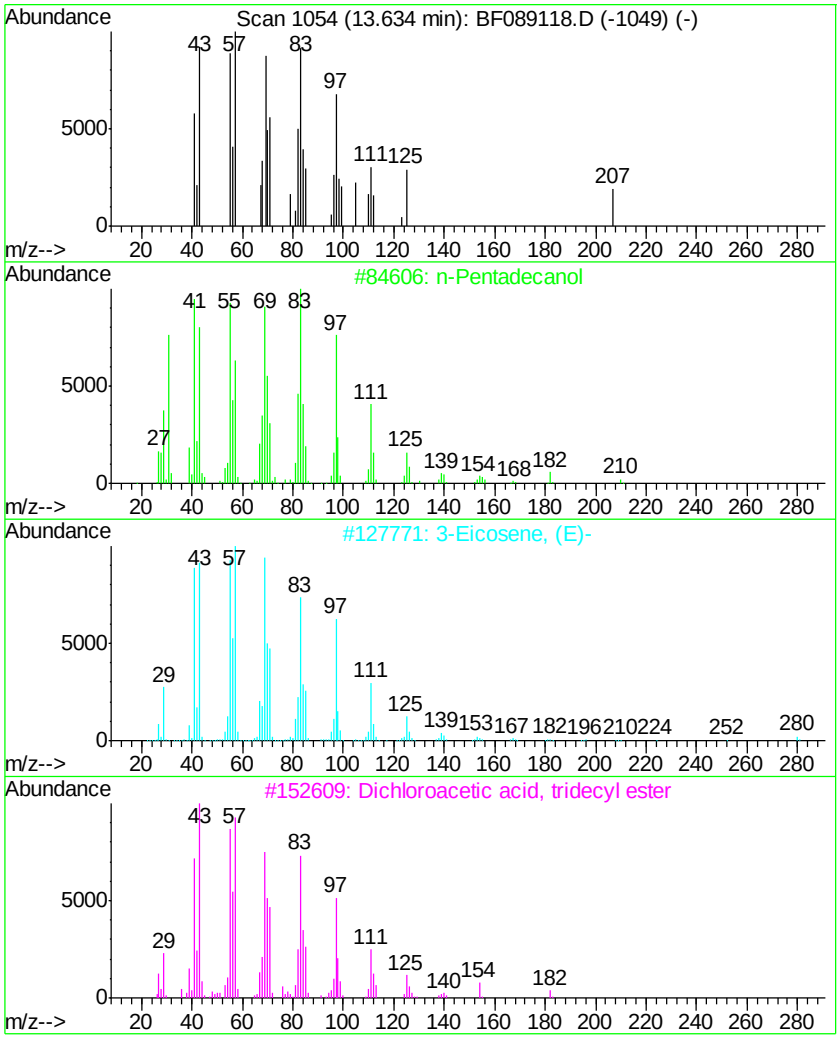
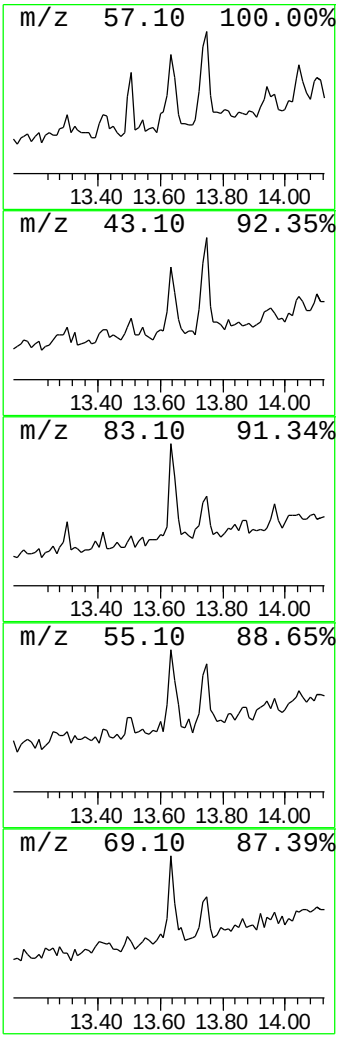
Peak Number 11 n-Pentadecanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.66 ng	44522	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Pentadecanol	228	C15H32O	000629-76-5	81
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	74
3	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	74
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	74
5	5-Tetradecanol acetate	256	C16H32O2	051354-25-7	74





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Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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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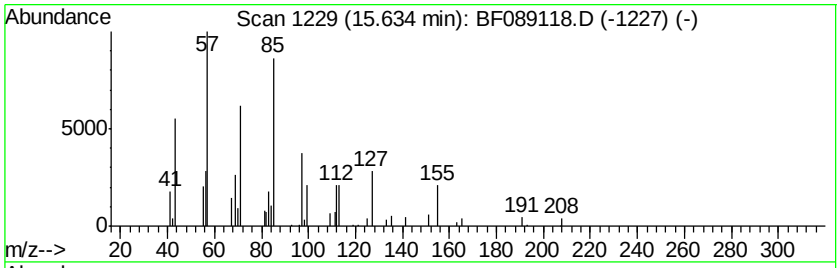
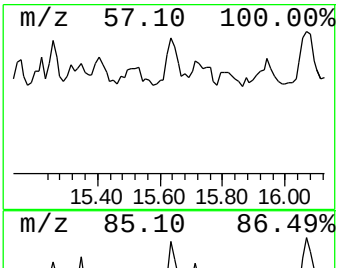
Peak Number 12 unknown15.63 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.19 ng	26520	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	47
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	43
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	43
4	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	38
5	Dodecane, 5-methyl-	184	C13H28	017453-93-9	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089118.D
Acq On : 19 Jul 2016 15:12
Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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

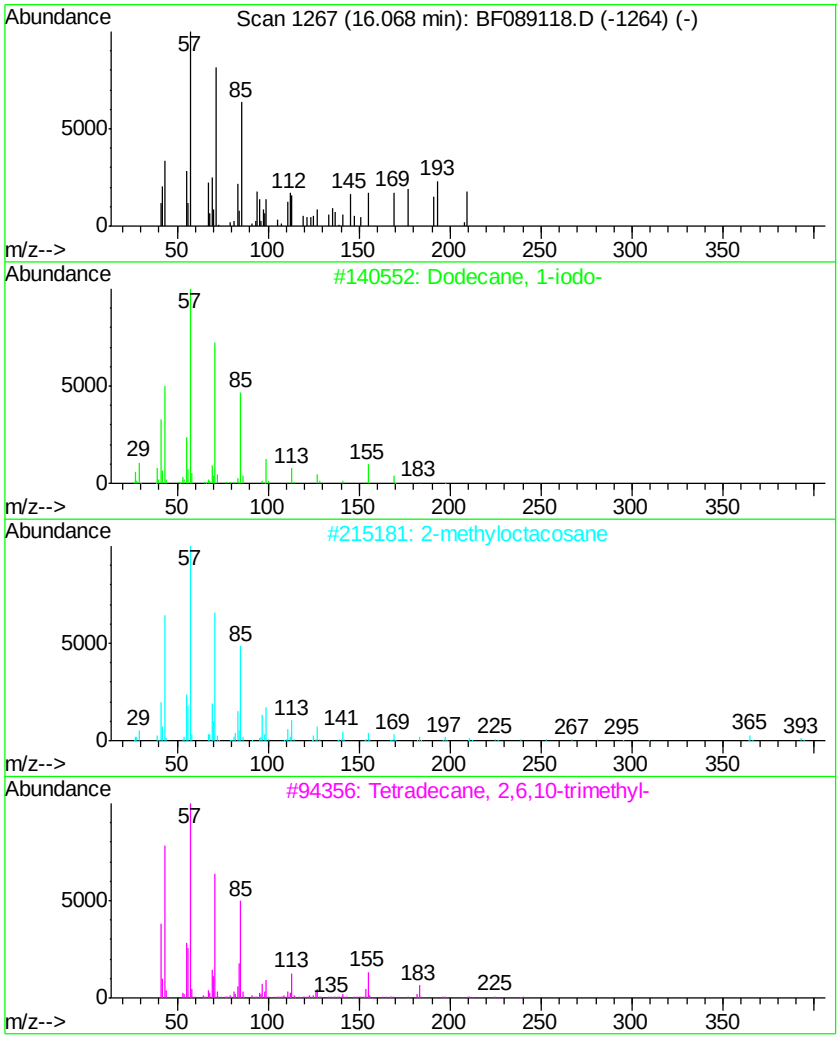
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

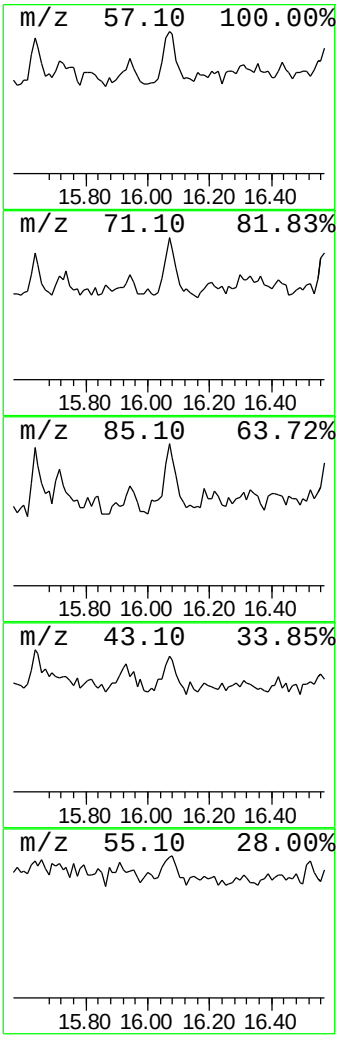
****

Peak Number 13 Dodecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.27 ng	39656	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50
2	2-methyloctacosane	408	C29H60	1000376-72-8	47
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	47
4	Pentadecane	212	C15H32	000629-62-9	47
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071916\
Data File : BF089118.D
Acq On : 19 Jul 2016 15:12
Operator : UM/SJ
Sample : H4071-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PO-001

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.10	2.10	3.3	ng	47216	1	6.62	282480	20.0
2,3-Butanediol	3.76	2.5	ng	35405	1	6.62	282480	20.0
3-Penten-2-one, 4...	4.02	64.4	ng	909862	1	6.62	282480	20.0
unknown4.54	4.54	4.4	ng	62030	1	6.62	282480	20.0
2-Pentanone, 4-hy...	4.76	62.9	ng	887979	1	6.62	282480	20.0
2-Pentanone, 4-me...	5.61	11.5	ng	162323	1	6.62	282480	20.0
unknown6.39	6.39	18.7	ng	264058	1	6.62	282480	20.0
2,4,6-Trichlorobe...	11.71	2.0	ng	36235	4	11.13	353846	20.0
n-Pentadecanol	13.63	2.7	ng	44522	5	13.75	334969	20.0
unknown15.63	15.63	2.2	ng	26520	6	15.10	242731	20.0
Dodecane, 1-iodo-	16.07	3.3	ng	39656	6	15.10	242731	20.0