LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041117\
Data File : BF094358.D
Acq On : 11 Apr 2017 18:56
Operator : SJ/MA
Sample : I2616-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

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-BF032217.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	2.058	14	29	31	rBV4	6460048	23927663	100.00%	29.849%
2	3.034	190	195	200	rBV	871884	901686	3.77%	1.125%
3	3.210	222	225	232	rVB	249135	278622	1.16%	0.348%
4	3.563	276	285	289	rBV	5257463	8932439	37.33%	11.143%
5	3.981	351	356	364	rVB	242476	344619	1.44%	0.430%
6	4.081	364	373	376	rBV	7126633	13596742	56.82%	16.961%
7	4.222	392	397	403	rVB	310189	305740	1.28%	0.381%
8	4.375	420	423	431	rVB	1162642	1033548	4.32%	1.289%
9	5.446	601	605	617	rVB	2011322	2118577	8.85%	2.643%
10	5.575	623	627	634	rVB	2176769	2097584	8.77%	2.617%
11	5.822	665	669	671	rBV	901501	878678	3.67%	1.096%
12	5.840	671	672	676	rVB	468428	375372	1.57%	0.468%
13	6.004	695	700	702	rBV	2711191	3804755	15.90%	4.746%
14	6.022	702	703	706	rVB	2575859	1304583	5.45%	1.627%
15	6.475	773	780	783	rBV	2064393	2488397	10.40%	3.104%
16	6.616	799	804	807	rBV	817189	799737	3.34%	0.998%
17	7.257	907	913	917	rBV	297255	321861	1.35%	0.402%
18	7.328	917	925	928	rBV	1048663	1140821	4.77%	1.423%
19	8.651	1143	1150	1153	rVB	3841626	4546149	19.00%	5.671%
20	9.463	1282	1288	1293	rBV2	1206824	1298787	5.43%	1.620%
21	10.439	1448	1454	1458	rBV	1525503	1684579	7.04%	2.101%
22	11.286	1592	1598	1602	rBV2	1217120	1670445	6.98%	2.084%
23	12.304	1766	1771	1778	rVB	643901	617007	2.58%	0.770%
24	13.274	1928	1936	1939	rBV	2996973	3604145	15.06%	4.496%
25	14.539	2146	2151	2155	rBV	1040759	1024996	4.28%	1.279%
26	16.168	2423	2428	2434	rBV	631232	723550	3.02%	0.903%
27	16.751	2521	2527	2532	rBV	243665	341417	1.43%	0.426%

Sum of corrected areas: 80162499

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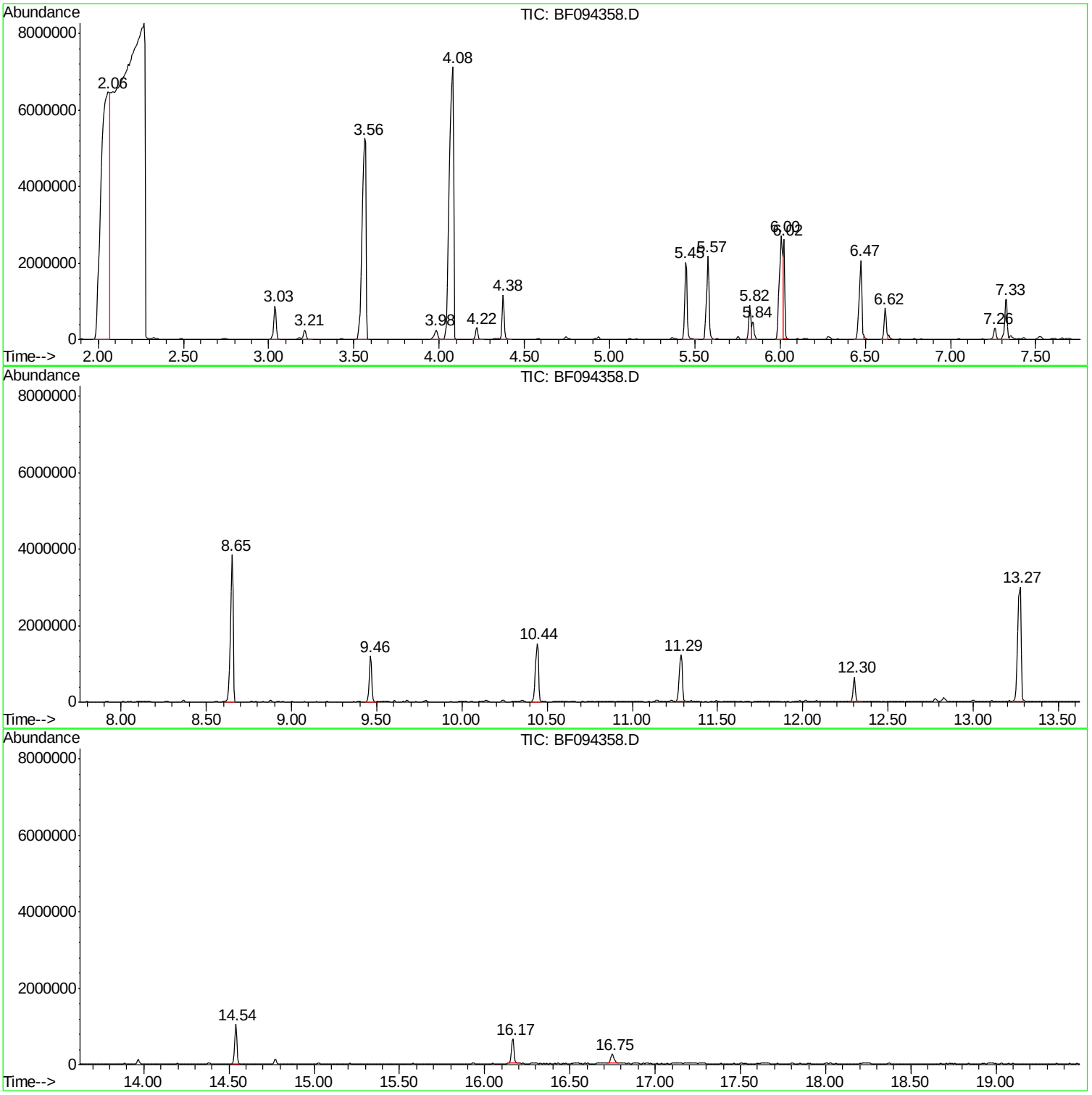
Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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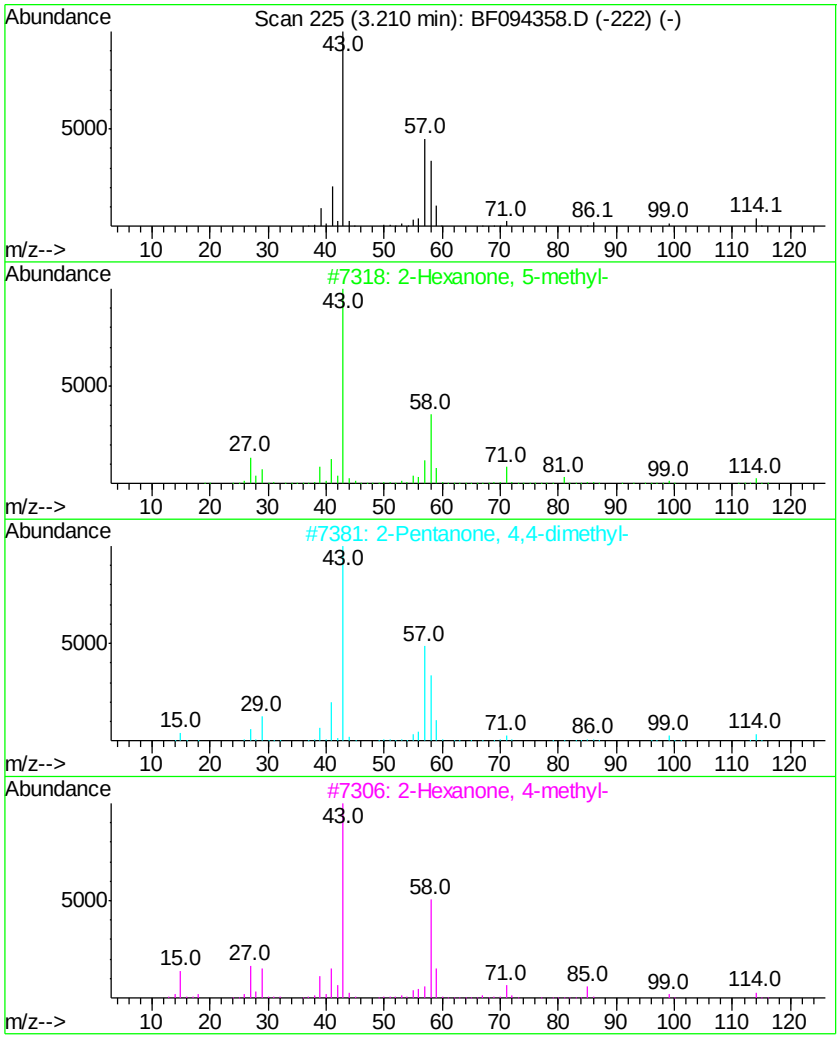
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

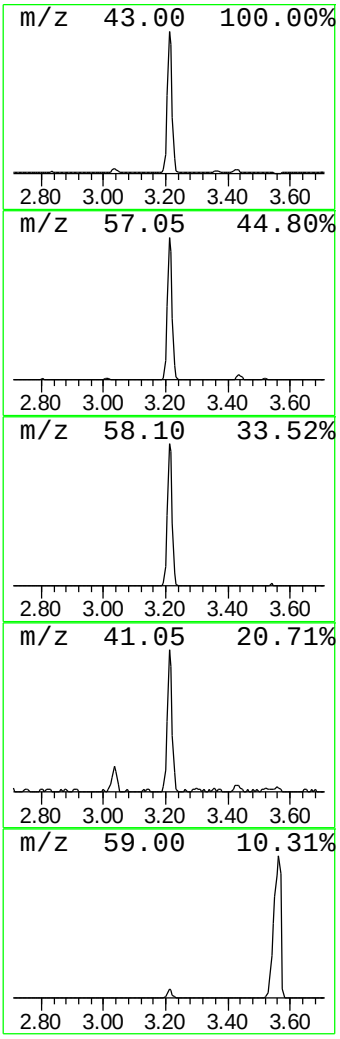
****

Peak Number 3 2-Hexanone, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	6.34 ng	278622	1,4-Dichlorobenzene-d4	5.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
2	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	64
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	59
4	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	40
5	2-Heptanone	114	C7H14O	000110-43-0	38





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Operator : SJ/MA
Sample : I2616-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

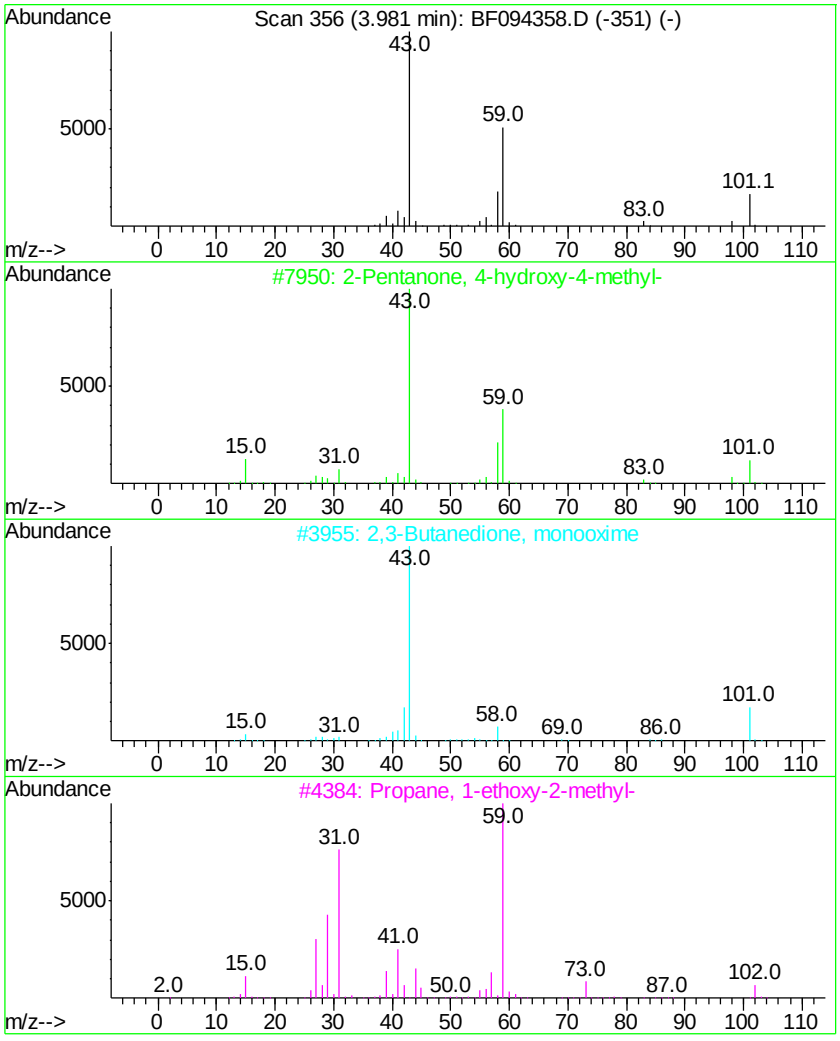
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

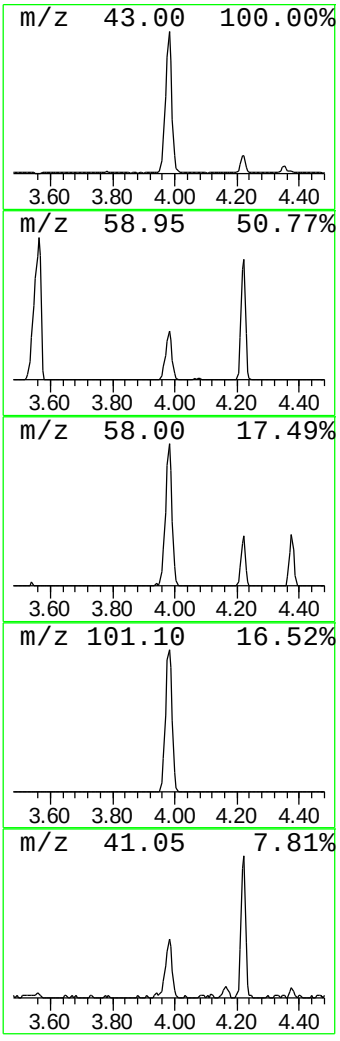
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	7.84 ng	344619	1,4-Dichlorobenzene-d4	5.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





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Operator : SJ/MA
Sample : I2616-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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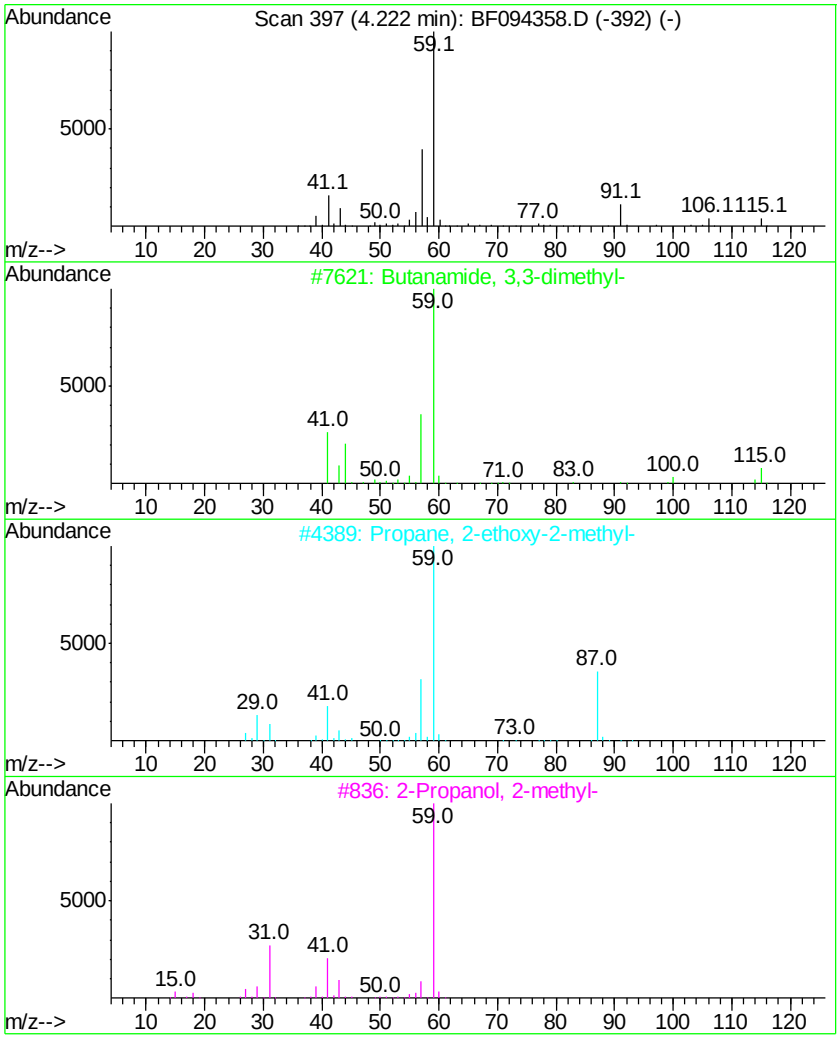
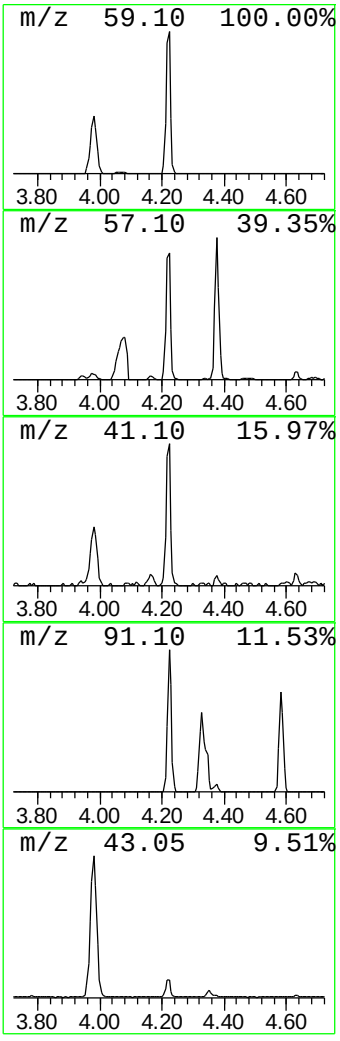
Peak Number 7 Butanamide, 3,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.22	6.96 ng	305740	1,4-Dichlorobenzene-d4	5.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	59
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	36
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Operator : SJ/MA
Sample : I2616-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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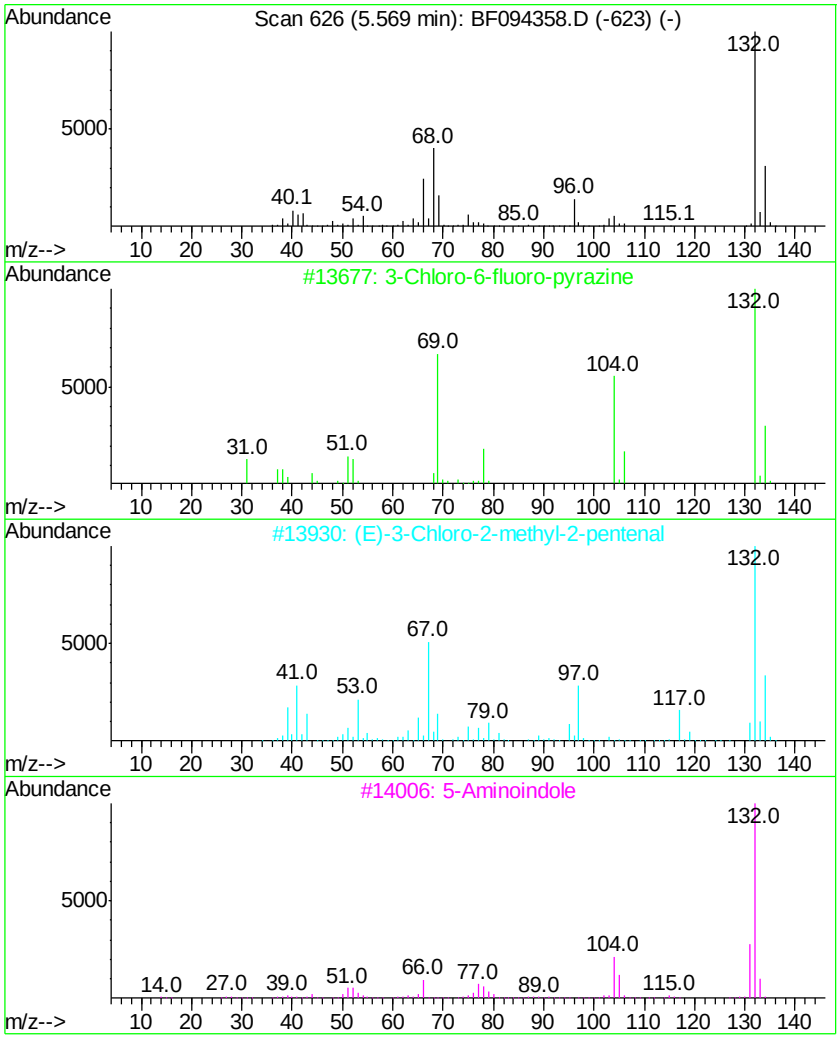
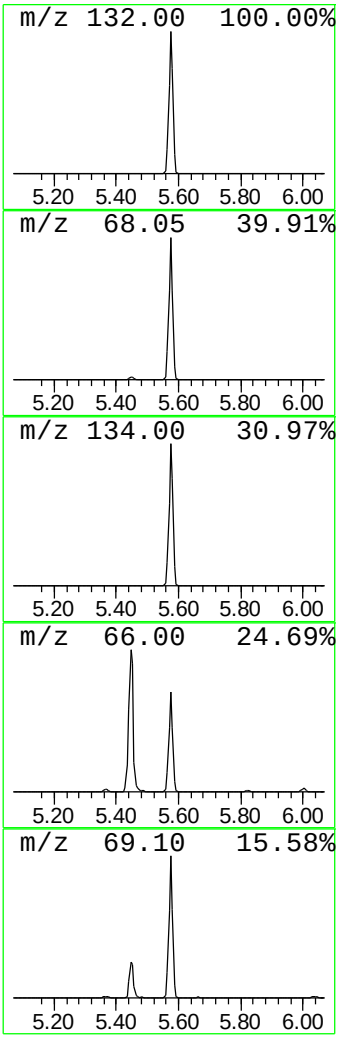
Peak Number 8 unknown5.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.57	47.74 ng	2097580	1,4-Dichlorobenzene-d4	5.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041117\
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Acq On : 11 Apr 2017 18:56
Operator : SJ/MA
Sample : I2616-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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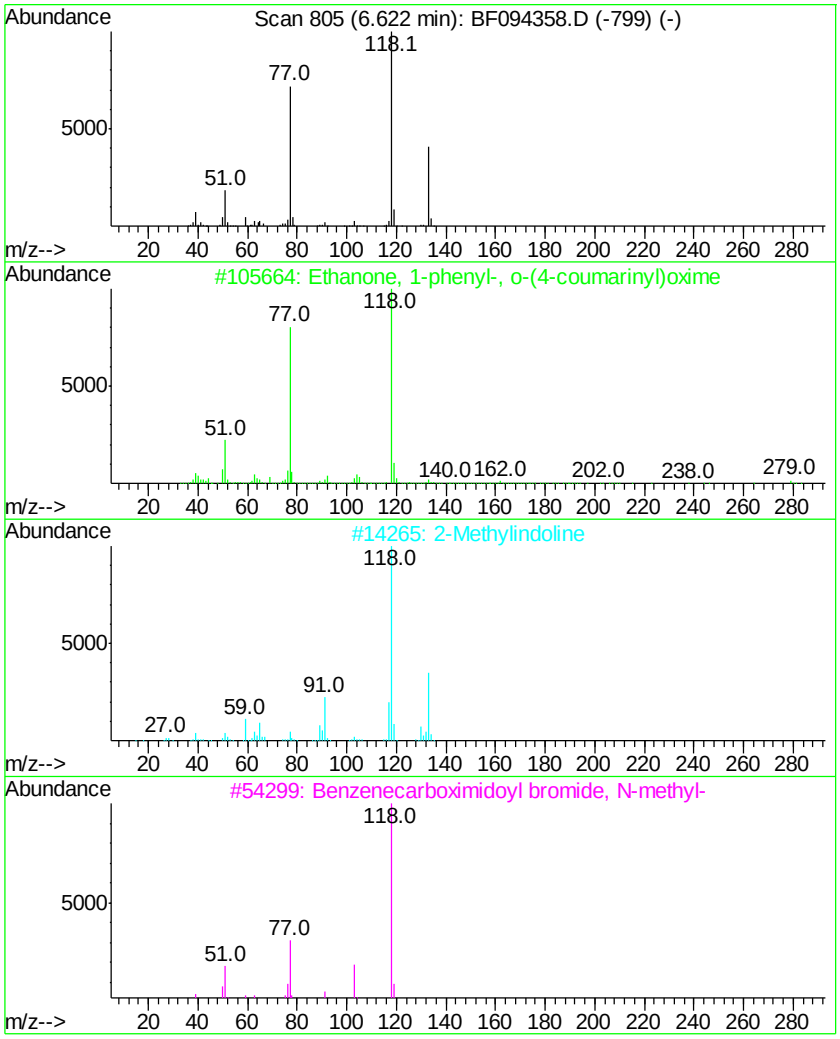
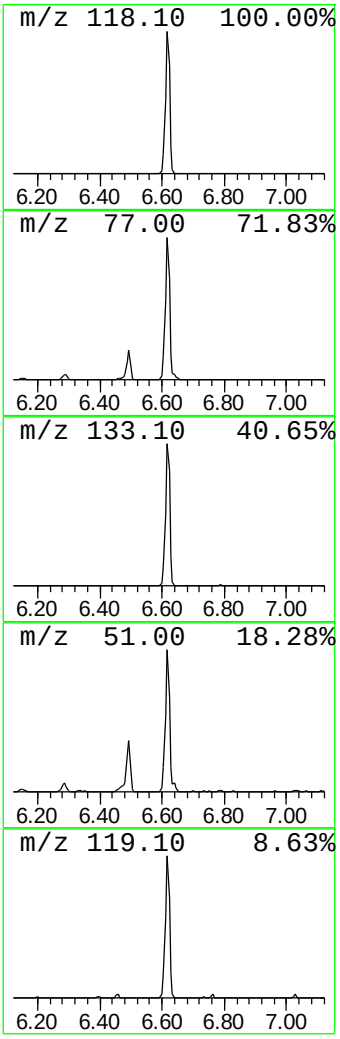
Peak Number 9 unknown6.62 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	14.02 ng	799737	Naphthalene-d8	7.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-phenyl-, o-(4-coumar...	279	C17H13NO3	034605-11-3	45
2	2-Methylindoline	133	C9H11N	006872-06-6	43
3	Benzenecarboximidoyl bromide, N-...	197	C8H8BrN	041182-85-8	32
4	Benzofuran	118	C8H6O	000271-89-6	12
5	Cyanic acid, phenyl ester	119	C7H5NO	001122-85-6	10





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FW2D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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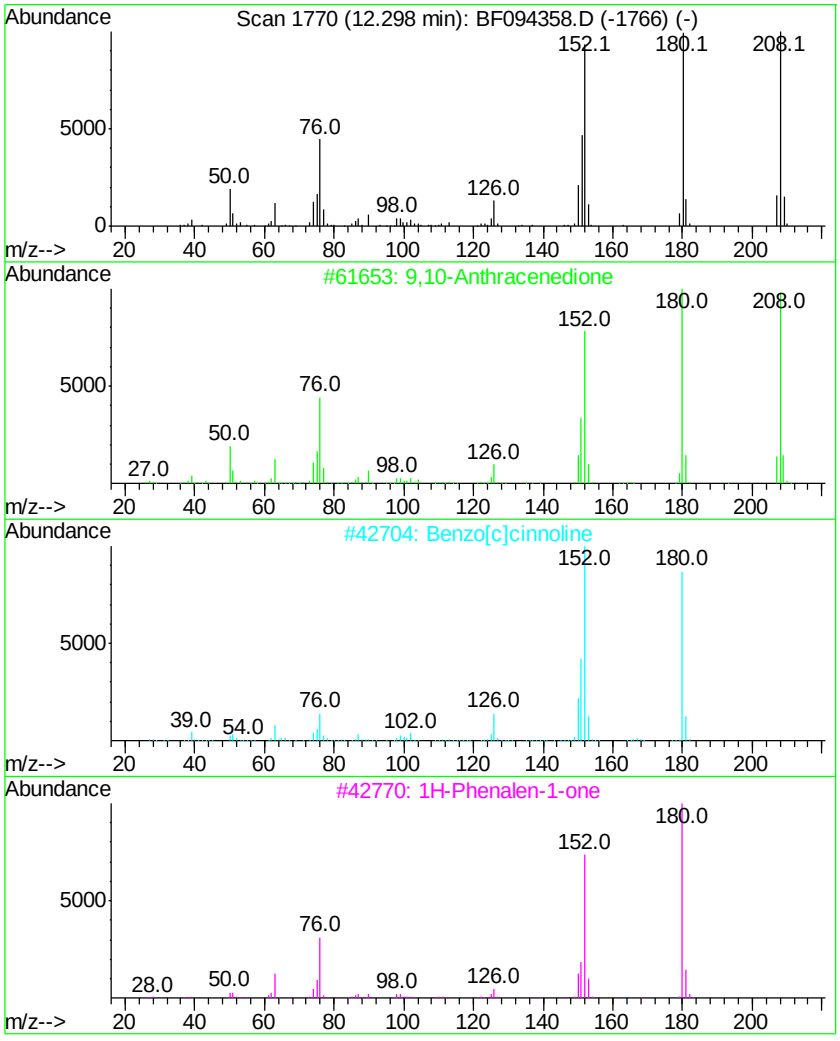
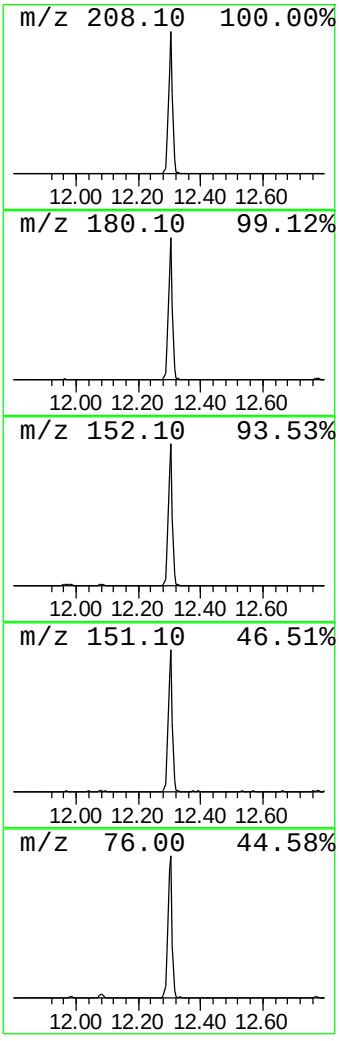
Peak Number 10 9,10-Anthracenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	7.39 ng	617007	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	86
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
4	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	60
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	58





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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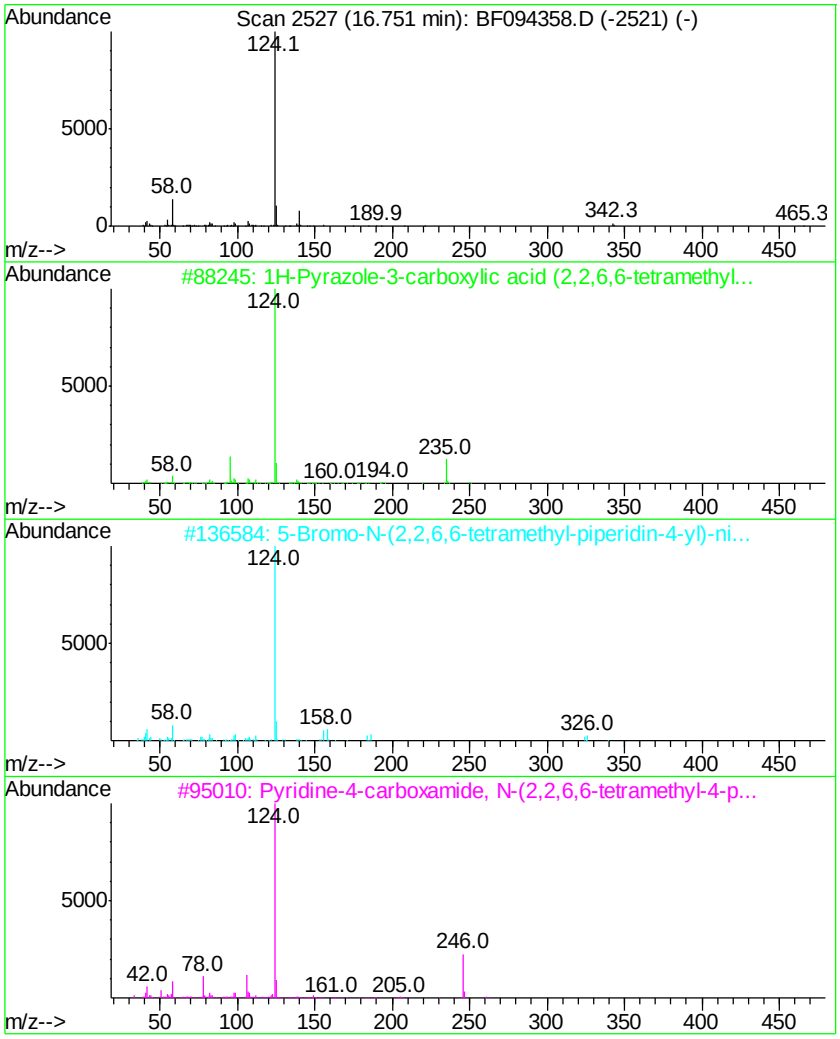
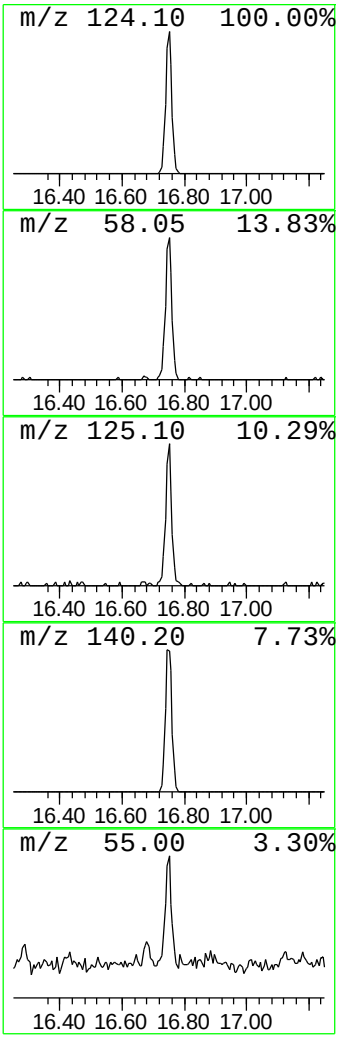
Peak Number 11 1H-Pyrazole-3-carboxylic ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	9.44 ng	341417	Perylene-d12	16.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-3-carboxylic acid (2...	250	C13H22N4O	1000296-44-0	50
2	5-Bromo-N-(2,2,6,6-tetramethyl-p...	339	C15H22BrN3O	1000295-18-6	40
3	Pyridine-4-carboxamide, N-(2,2,6...	261	C15H23N3O	1000273-73-9	39
4	Decanedioic acid, bis(2,2,6,6-te...	480	C28H52N2O4	052829-07-9	37
5	Benzoic acid, 2,2,6,6-tetramethy...	261	C16H23NO2	026275-88-7	32





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
2-Hexanone, 5-met...	3.21	6.3	ng	278622	1	5.82	878678	20.0
2-Pentanone, 4-hy...	3.98	7.8	ng	344619	1	5.82	878678	20.0
Butanamide, 3,3-d...	4.22	7.0	ng	305740	1	5.82	878678	20.0
unknown5.57	5.57	47.7	ng	2097580	1	5.82	878678	20.0
unknown6.62	6.62	14.0	ng	799737	2	7.33	1140820	20.0
9,10-Anthracenedione	12.30	7.4	ng	617007	4	11.29	1670450	20.0
1H-Pyrazole-3-car...	16.75	9.4	ng	341417	6	16.17	723550	20.0