LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072916\
Data File : BF089375.D
Acq On : 28 Jul 2016 21:16
Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

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-BF072716.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	1.678	7	8	44	rVB	1344269	2982105	100.00%	65.137%
2	6.296	409	412	414	rBV	19500	33383	1.12%	0.729%
3	6.456	414	426	427	rVV	90359	386292	12.95%	8.438%
4	6.524	427	432	441	rVV	133544	458441	15.37%	10.014%
5	10.570	784	786	791	rBB	60771	55439	1.86%	1.211%
6	10.971	819	821	825	rVB	98223	142078	4.76%	3.103%
7	11.576	872	874	884	rVB	86811	110845	3.72%	2.421%
8	11.931	903	905	907	rBV	43424	56537	1.90%	1.235%
9	11.965	907	908	918	rVB2	95298	168477	5.65%	3.680%
10	13.062	999	1004	1006	rBV	33796	43904	1.47%	0.959%
11	13.199	1013	1016	1025	rVB	56263	92434	3.10%	2.019%
12	13.451	1034	1038	1042	rBV	29807	48258	1.62%	1.054%

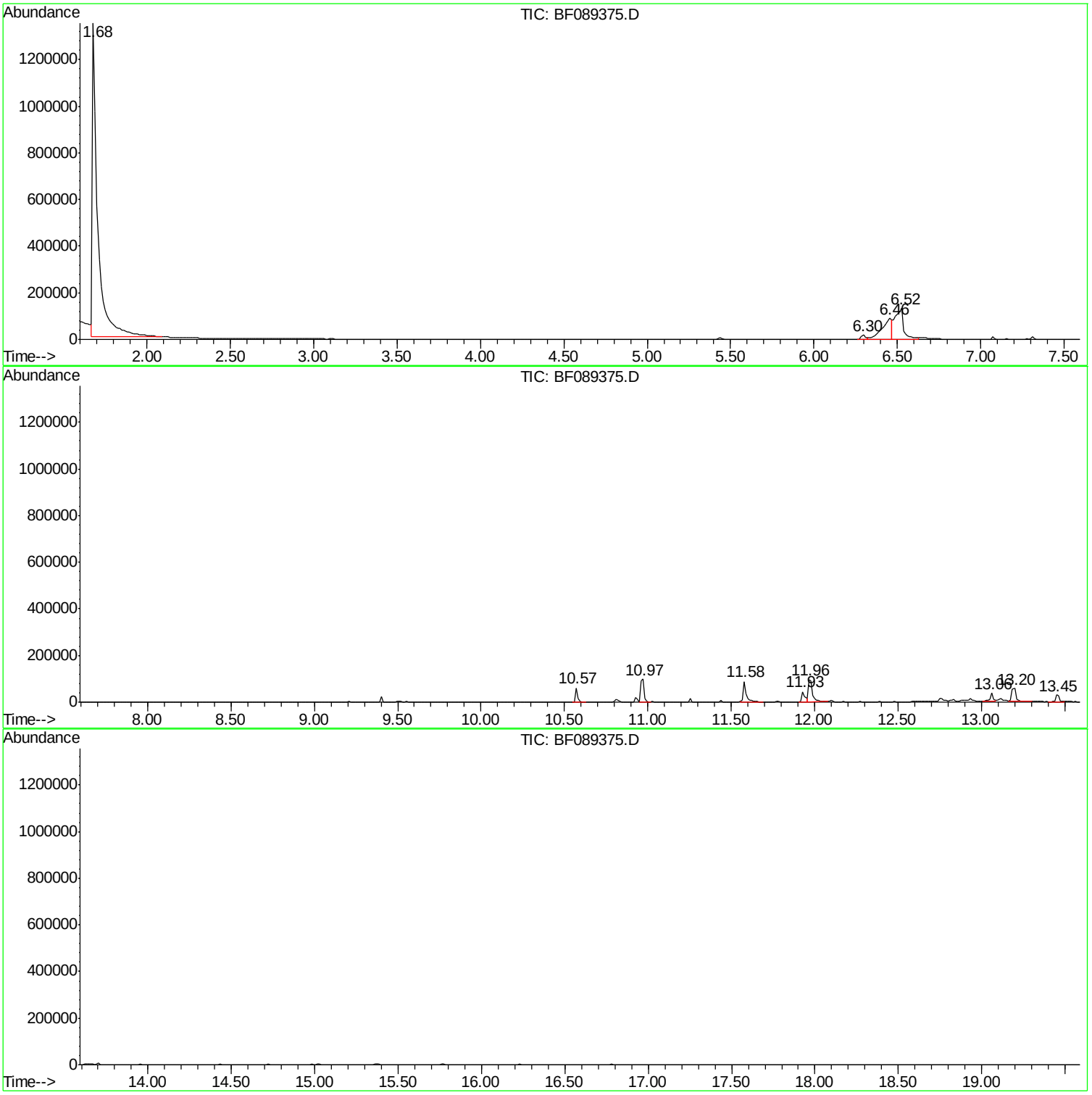
Sum of corrected areas: 4578193

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072916\
Data File : BF089375.D
Acq On : 28 Jul 2016 21:16
Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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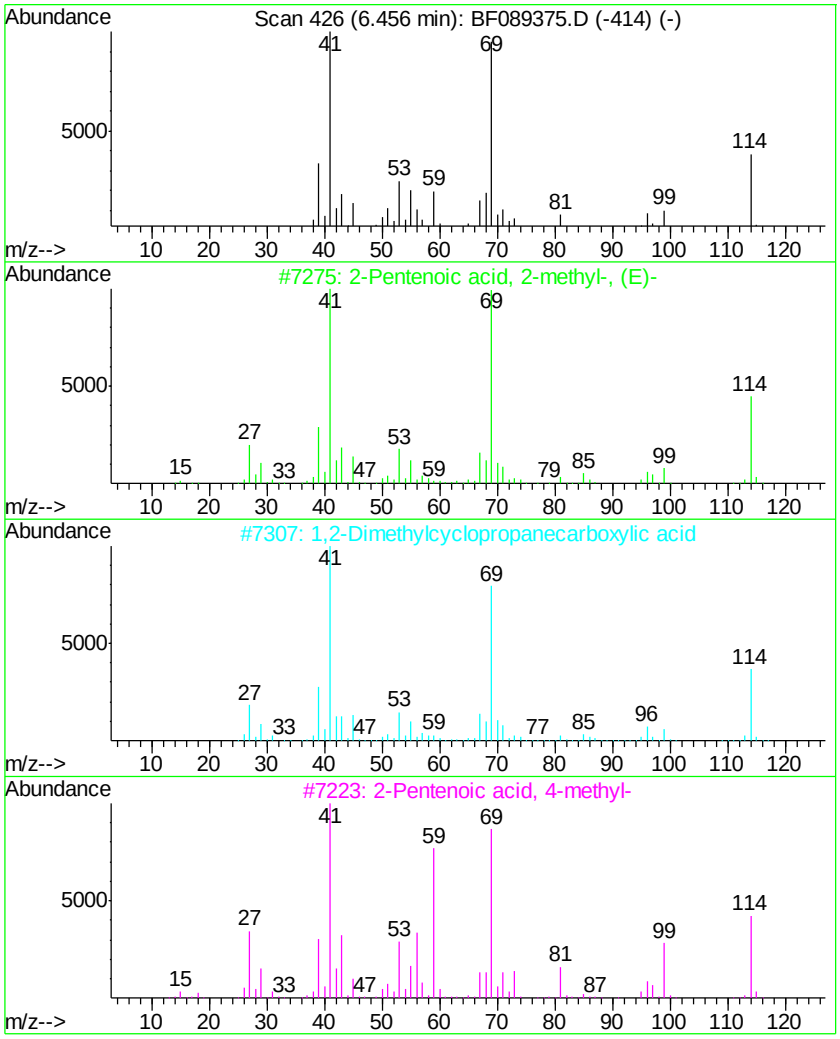
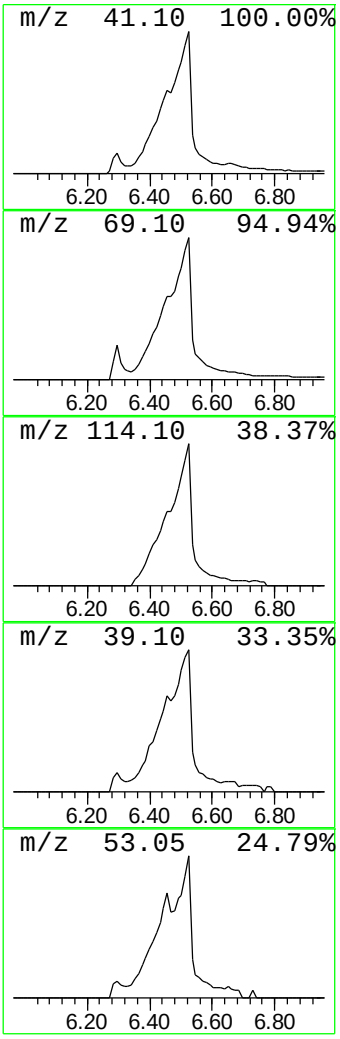
Peak Number 2 2-Pentenoic acid, 2-methyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	16.85 ng	386292	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenoic acid, 2-methyl-, (E)-	114	C6H10O2	016957-70-3	76
2	1,2-Dimethylcyclopropanecarboxyl...	114	C6H10O2	1000191-14-6	76
3	2-Pentenoic acid, 4-methyl-	114	C6H10O2	010321-71-8	64
4	2-Pentenoic acid, 2-methyl-	114	C6H10O2	003142-72-1	52
5	3-Hexenoic acid	114	C6H10O2	004219-24-3	50





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Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

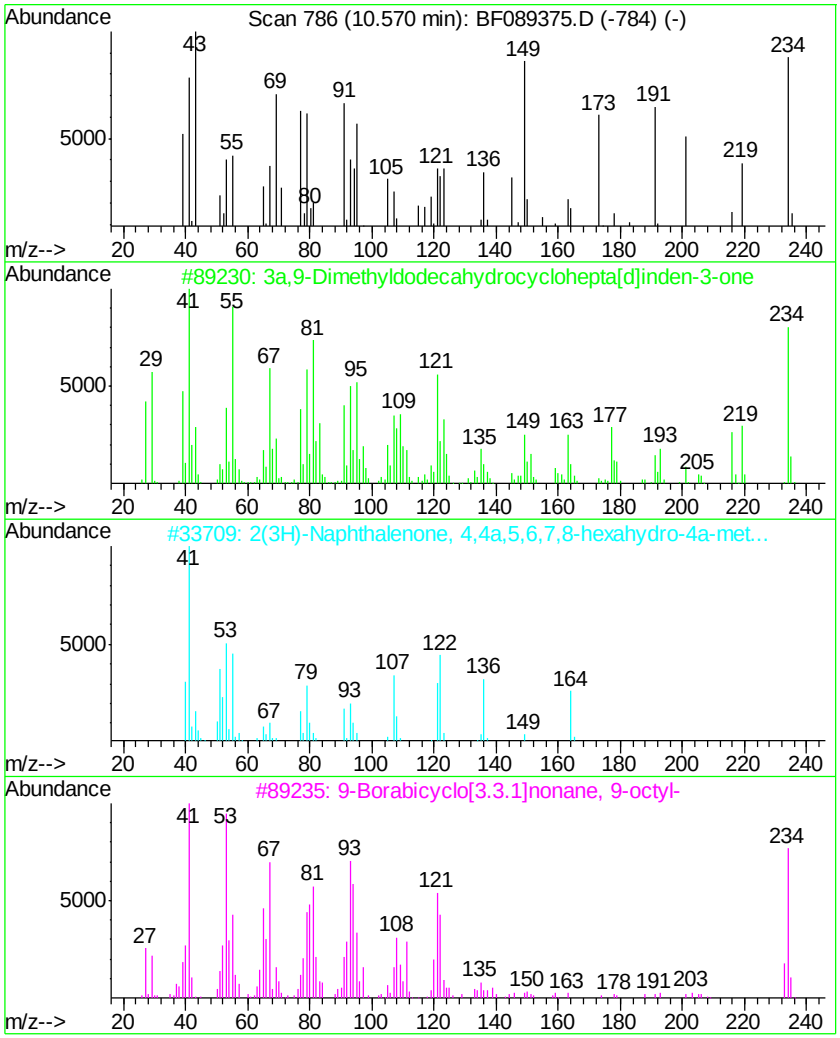
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

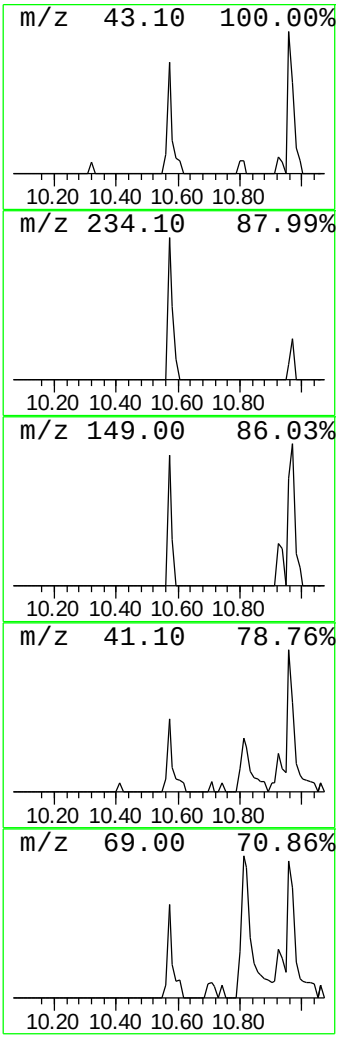
****

Peak Number 3 3a,9-Dimethyldodecahydrocyc... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	7.80 ng	55439	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3a,9-Dimethyldodecahydrocyclohep...	234	C16H26O	1000189-38-7	53
2	2(3H)-Naphthalenone, 4,4a,5,6,7,...	164	C11H16O	004087-39-2	35
3	9-Borabicyclo[3.3.1]nonane, 9-oc...	234	C16H31B	030089-00-0	27
4	(1S,6R,9S,10S)-5,5,9,10-Tetramet...	234	C16H26O	1000298-98-1	20
5	2-Isopropylidene-3-methylhexa-3,...	150	C10H14O	1000191-76-5	20





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Data File : BF089375.D
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Sample : H4200-03 50X
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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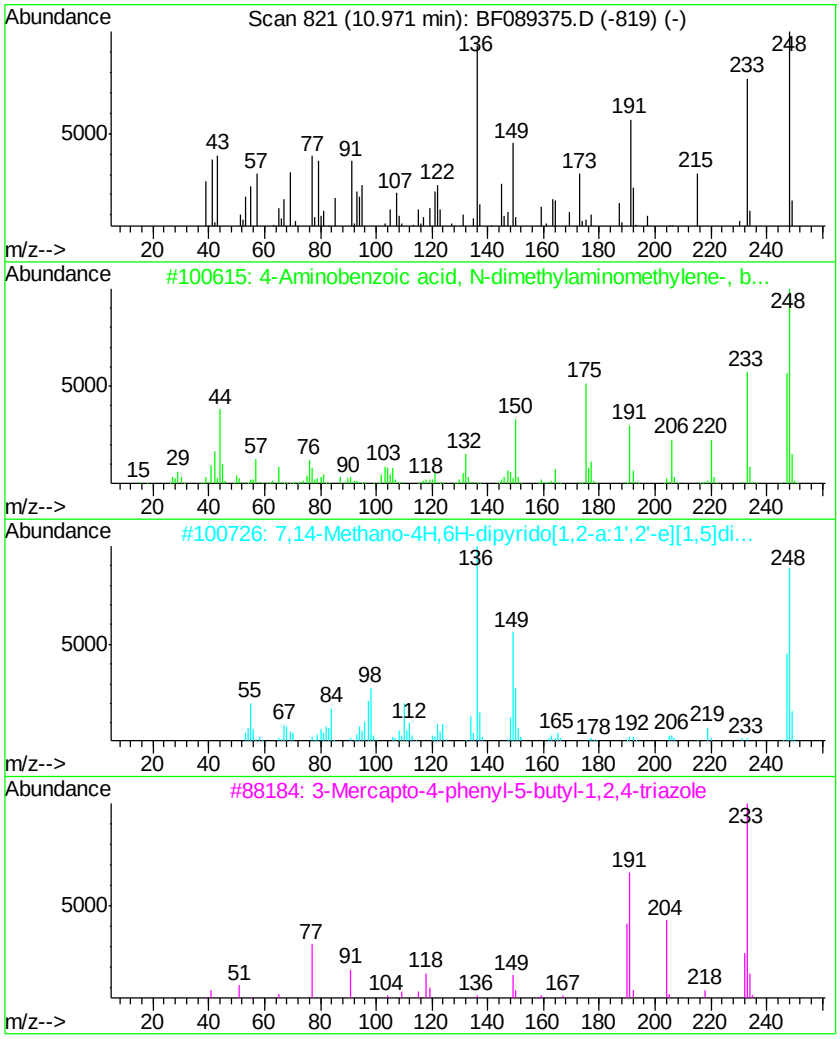
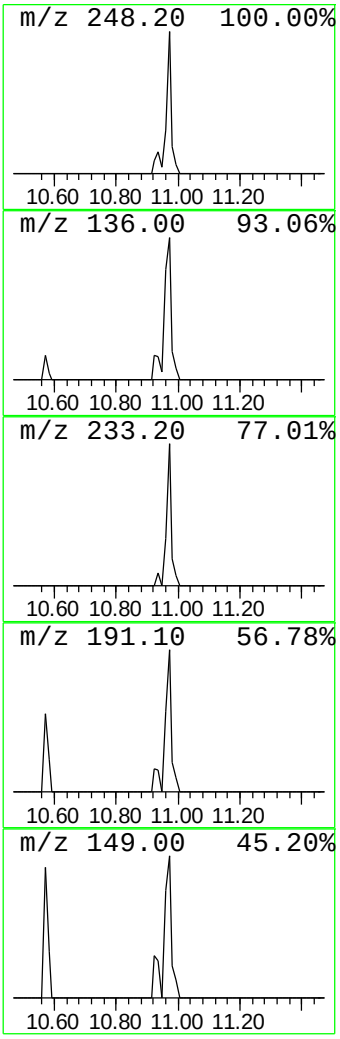
Peak Number 4 unknown10.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	20.00 ng	142078	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Aminobenzoic acid, N-dimethyla...	248	C14H20N2O2	1000375-81-5	43
2	7,14-Methano-4H,6H-dipyrido[1,2-...	248	C15H24N2O	000486-87-3	43
3	3-Mercapto-4-phenyl-5-butyl-1,2,...	233	C12H15N3S	066921-09-3	25
4	Pyrrole-2,5-dione, 1-(2,5-dimeth...	233	C12H11NO4	040783-24-2	25
5	4,5-Diphenyl-2-pyrone	248	C17H12O2	1000306-52-2	25





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Sample : H4200-03 50X
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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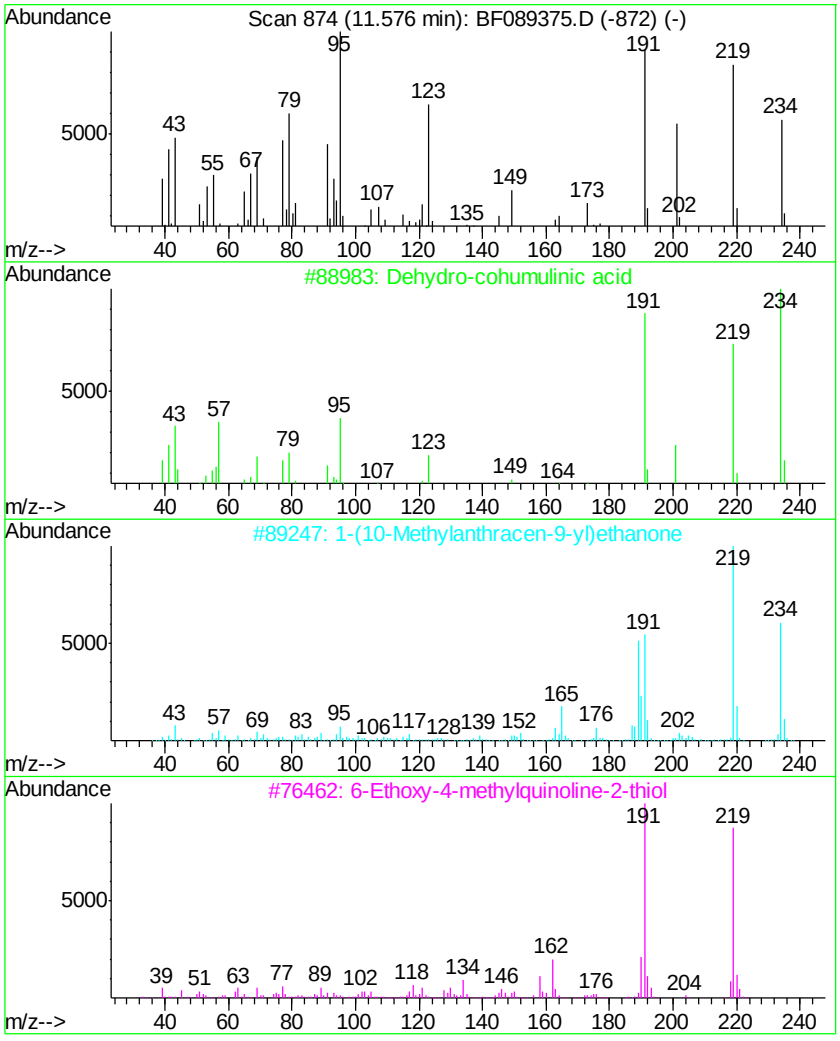
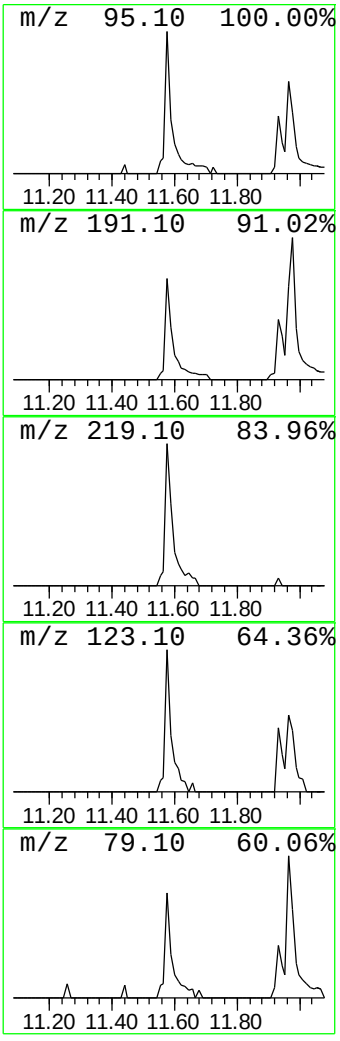
****

Peak Number 5 Dehydro-cohumulinic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	15.60 ng	110845	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydro-cohumulinic acid	234	C14H18O3	1000041-27-1	78
2	1-(10-Methylanthracen-9-yl)ethanone	234	C17H14O	036778-18-4	38
3	6-Ethoxy-4-methylquinoline-2-thiol	219	C12H13NOS	1000303-46-9	30
4	4H-1-Benzopyran-4-one, 3-acetyl-...	234	C12H10O5	001022-78-2	25
5	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	25





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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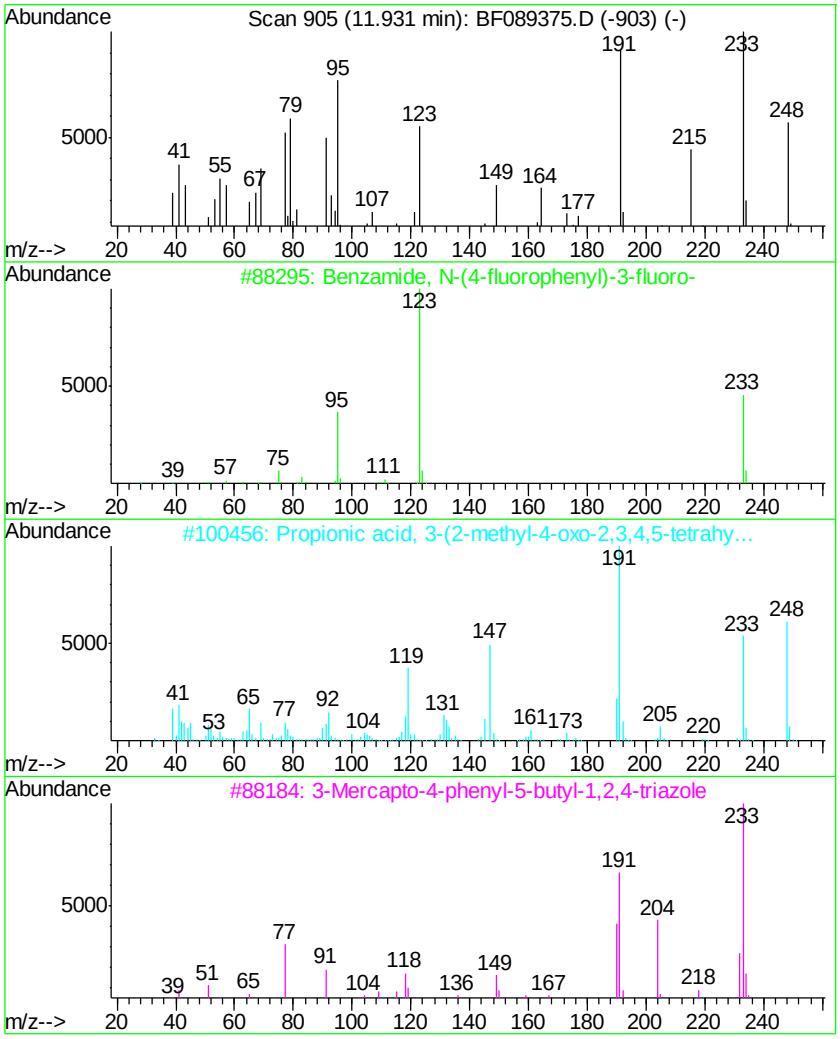
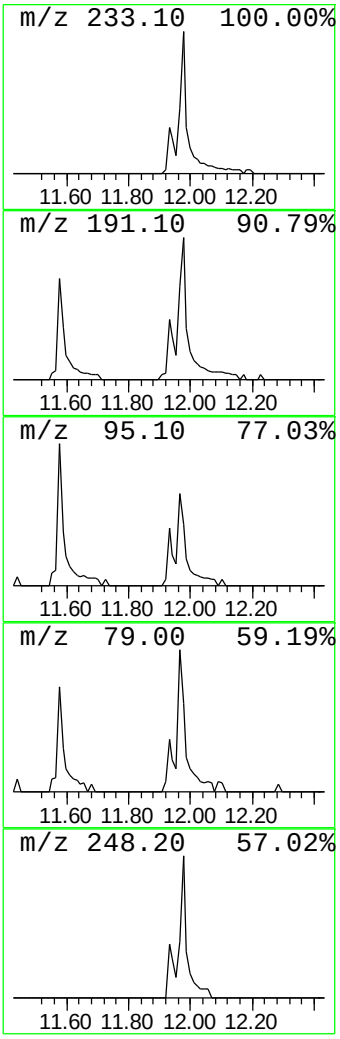
****

Peak Number 6 unknown11.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	7.96 ng	56537	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-(4-fluorophenyl)-3-...	233	C13H9F2NO	1000307-16-3	38
2	Propionic acid, 3-(2-methyl-4-ox...	248	C13H16N2O3	1000304-99-5	38
3	3-Mercapto-4-phenyl-5-butyl-1,2,...	233	C12H15N3S	066921-09-3	35
4	2,4,6-Triisopropylbenzoic acid	248	C16H24O2	049623-71-4	22
5	2(1H)-Pyrimidinethione, 3,4-dihy...	248	C13H16N2OS	063704-47-2	22





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Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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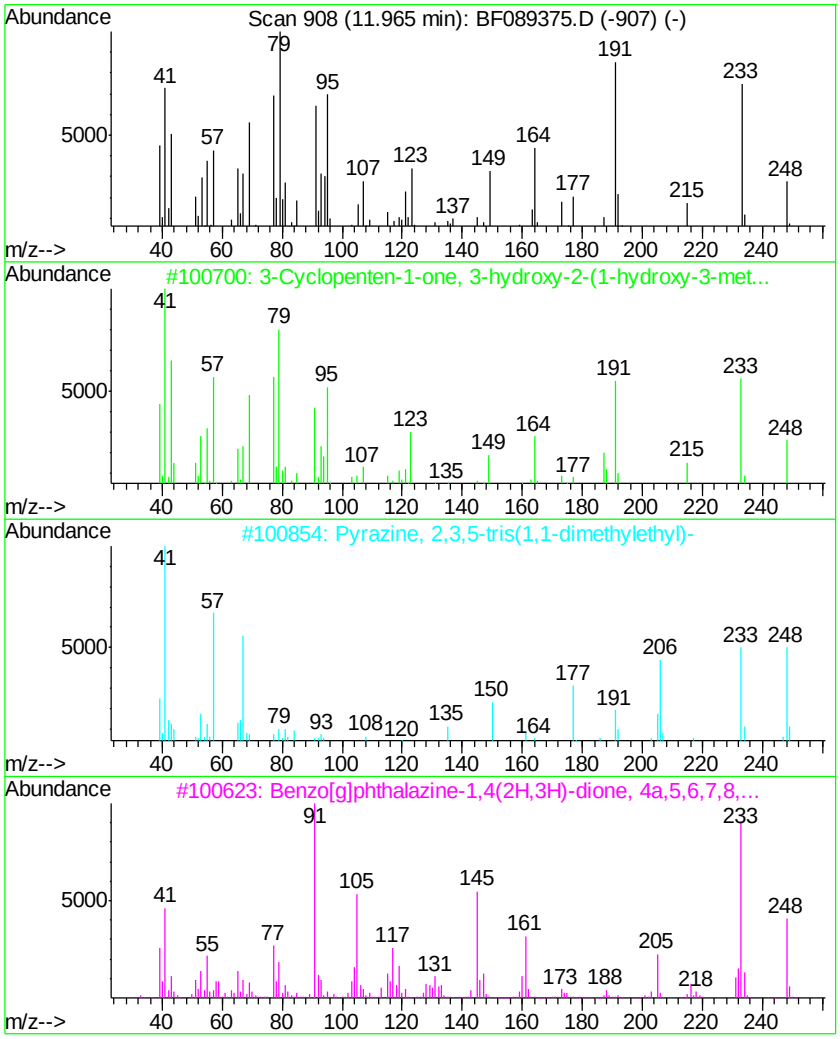
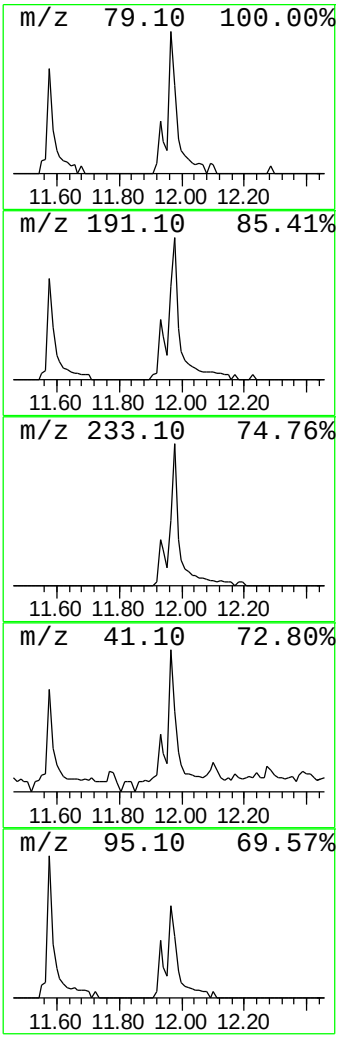
****

Peak Number 7 3-Cyclopenten-1-one, 3-hydr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	23.72 ng	168477	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclopenten-1-one, 3-hydroxy-2...	248	C15H20O3	038574-23-1	89
2	Pyrazine, 2,3,5-tris(1,1-dimethy...	248	C16H28N2	039950-98-6	25
3	Benzo[g]phthalazine-1,4(2H,3H)-d...	248	C14H20N2O2	326611-32-9	25
4	3-Mercapto-4-phenyl-5-butyl-1,2,...	233	C12H15N3S	066921-09-3	22
5	Pentanenitrile, 2-(4-fluoropheny...	233	C12H12FN3O	1000269-22-3	18





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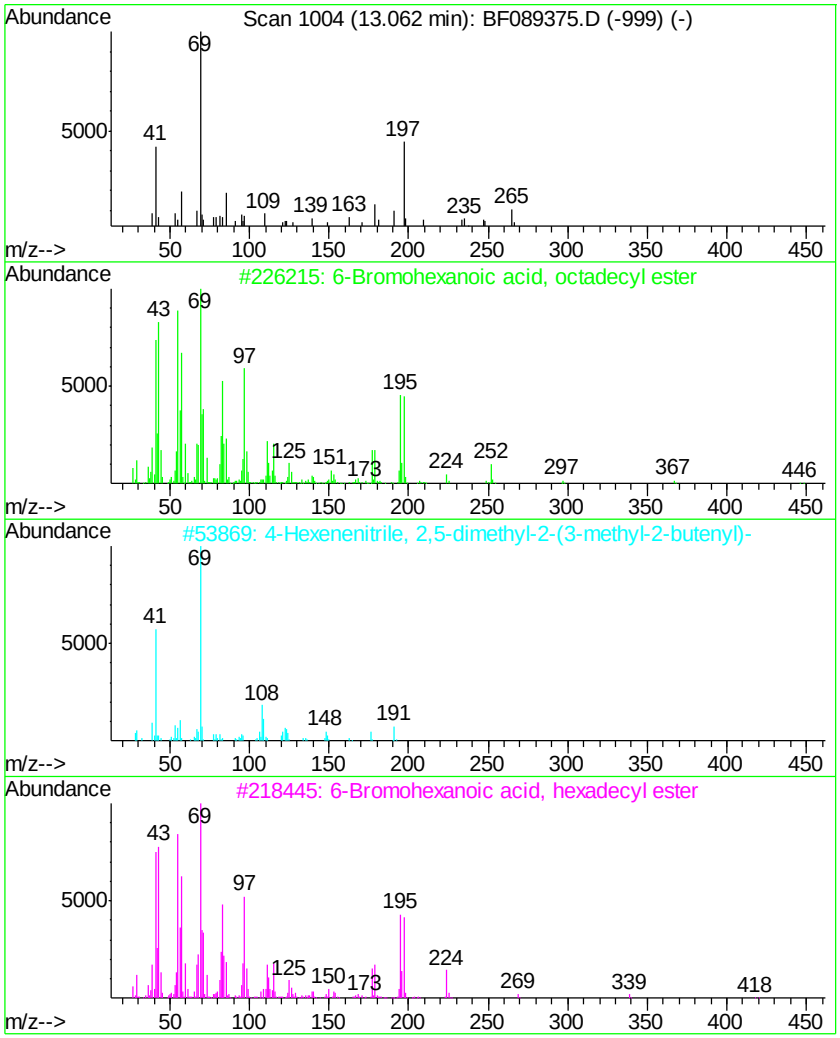
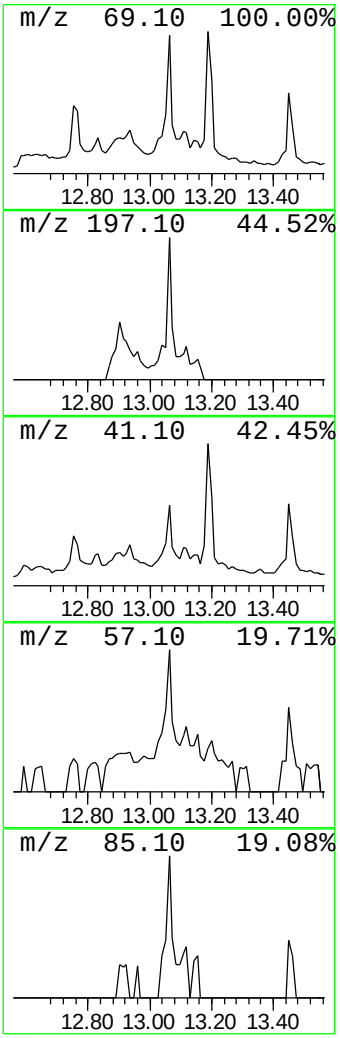
Peak Number 8 unknown13.06 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	18.20 ng	43904	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Bromohexanoic acid, octadecyl ...	446	C24H47BrO2	1000281-92-1	39
2	4-Hexenenitrile, 2,5-dimethyl-2-...	191	C13H21N	069340-56-3	38
3	6-Bromohexanoic acid, hexadecyl ...	418	C22H43BrO2	1000281-92-0	38
4	Cyclopropylcarboxylic acid, 2,4,...	264	C10H7Cl3O2	1000325-67-6	38
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	35





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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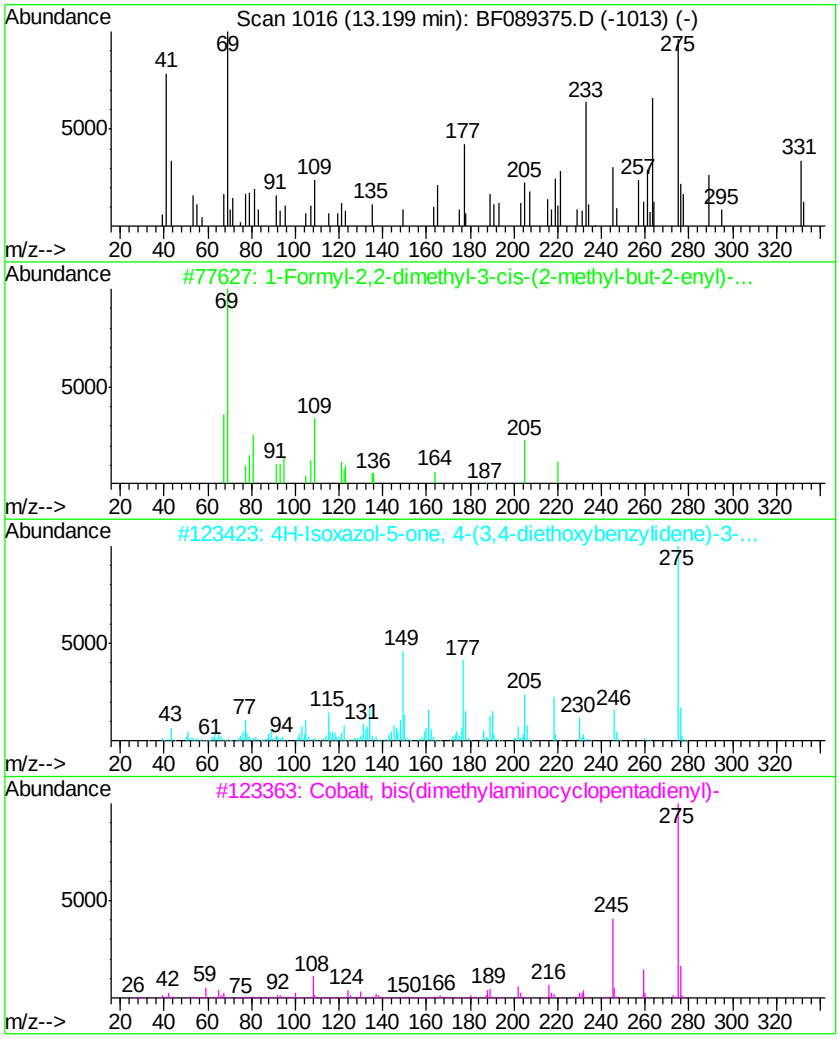
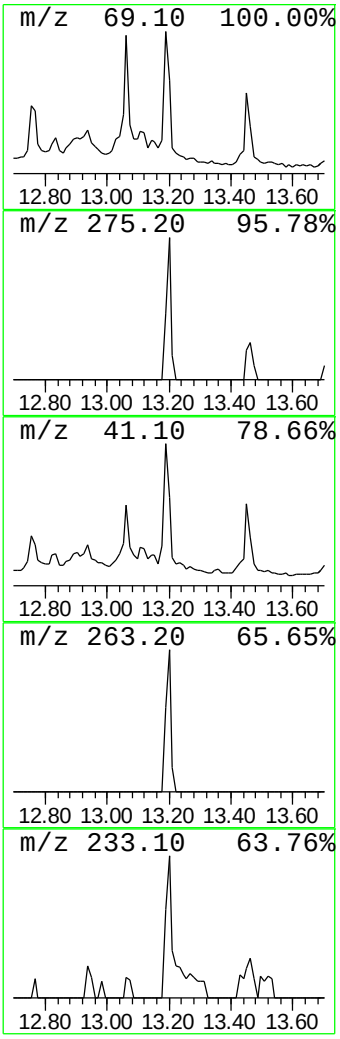
****

Peak Number 9 unknown13.20 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	38.31 ng	92434	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	45
2	4H-Isoxazol-5-one, 4-(3,4-dietho...	275	C15H17NO4	1000316-44-0	25
3	Cobalt, bis(dimethylaminocyclope...	275	C14H20CoN2	1000162-00-1	14
4	1H-Pyrazolo[4',3':5,6]pyrido[2,3...	275	C12H13N5O3	349496-02-2	11
5	Phenol, o-(2,4-dinitroanilino)-	275	C12H9N3O5	006358-23-2	11





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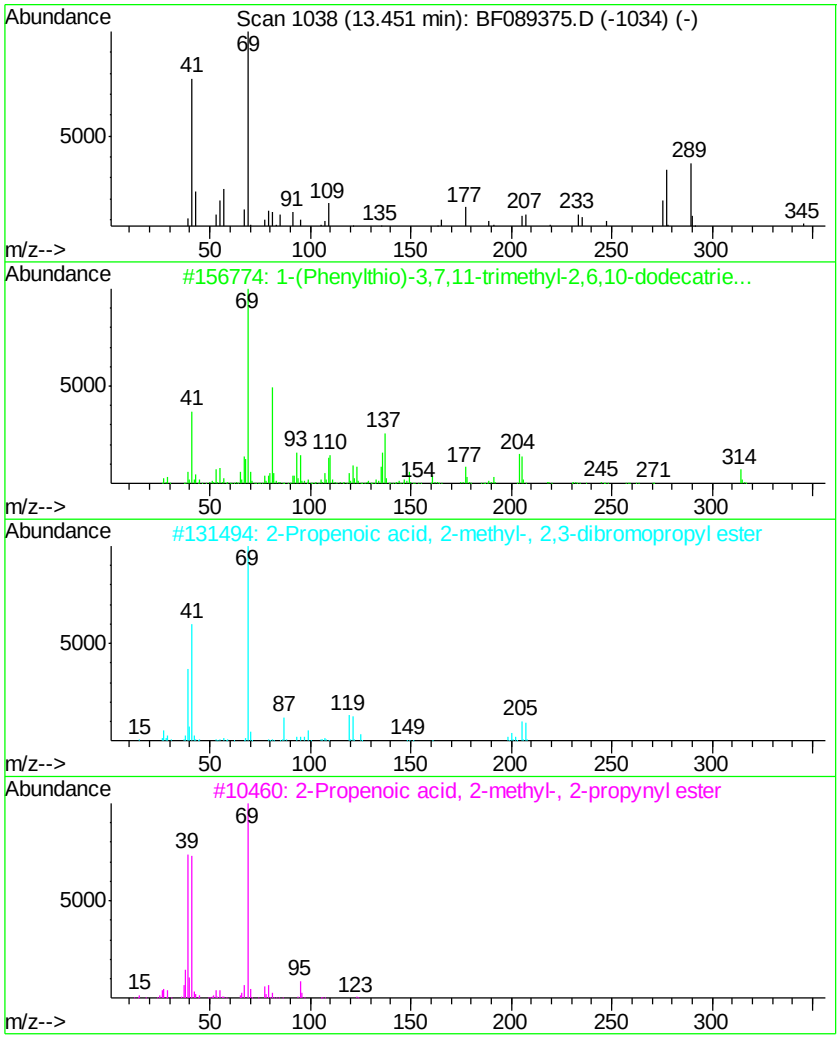
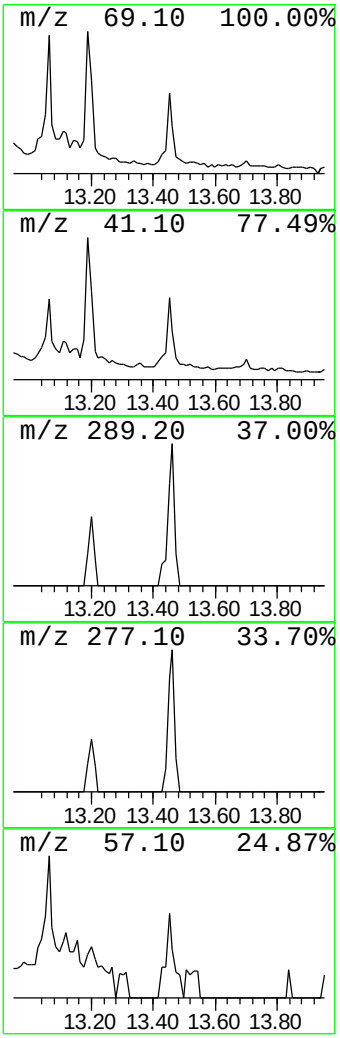
Peak Number 10 unknown13.45 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	20.00 ng	48258	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	25
2	2-Propenoic acid, 2-methyl-, 2,3...	284	C7H10Br2O2	003066-70-4	17
3	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	17
4	1-Propyne, 3-(2-bromoethoxy)-	162	C5H7BrO	018668-74-1	17
5	1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	17





Tentatively Identified Compound (LSC) summary

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Acq On : 28 Jul 2016 21:16
Operator : UM/SJ
Sample : H4200-03 50X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1607134563-67(COMPO)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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
2-Pentenoic acid,...	6.46	16.9	ng	386292	1	6.54	458441	20.0
3a,9-Dimethyldode...	10.57	7.8	ng	55439	4	11.03	142078	20.0
unknown10.97	10.97	20.0	ng	142078	4	11.03	142078	20.0
Dehydro-cohumulin...	11.58	15.6	ng	110845	4	11.03	142078	20.0
unknown11.93	11.93	8.0	ng	56537	4	11.03	142078	20.0
3-Cyclopenten-1-o...	11.96	23.7	ng	168477	4	11.03	142078	20.0
unknown13.06	13.06	18.2	ng	43904	5	13.66	48258	20.0
unknown13.20	13.20	38.3	ng	92434	5	13.66	48258	20.0
unknown13.45	13.45	20.0	ng	48258	5	13.66	48258	20.0