LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087804.D
Acq On : 8 Jun 2016 00:17
Operator : UM/SJ
Sample : H3379-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-7

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF087805.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.701	6	10	12	rVB	3953078	6108613	100.00%	19.536%
2	1.758	14	15	25	rVV	318032	500442	8.19%	1.600%
3	1.895	25	27	43	rVB	1312803	2338685	38.29%	7.479%
4	2.101	43	45	61	rVB	69241	190171	3.11%	0.608%
5	3.164	135	138	151	rBV	40960	98279	1.61%	0.314%
6	5.027	298	301	307	rBV	185182	257431	4.21%	0.823%
7	5.439	334	337	340	rBV	1911403	2369800	38.79%	7.579%
8	6.479	425	428	430	rBV	2222325	2515436	41.18%	8.045%
9	6.616	437	440	442	rBV	1891581	2699760	44.20%	8.634%
10	6.844	457	460	462	rBV	530846	565487	9.26%	1.808%
11	6.993	471	473	476	rVB	1559110	2014334	32.98%	6.442%
12	7.404	506	509	512	rBV	1491117	1547982	25.34%	4.951%
13	8.125	570	572	574	rBV	943513	775490	12.70%	2.480%
14	9.199	663	666	669	rBV	2355119	2592495	42.44%	8.291%
15	9.599	698	701	703	rBV	501615	543737	8.90%	1.739%
16	9.873	723	725	728	rVB	941088	806895	13.21%	2.580%
17	10.662	791	794	796	rBV	1676952	1621427	26.54%	5.185%
18	11.348	852	854	857	rBV2	584755	679707	11.13%	2.174%
19	12.936	990	993	995	rBV	2043725	1863962	30.51%	5.961%
20	13.851	1070	1073	1077	rBV	47280	91325	1.50%	0.292%
21	13.977	1081	1084	1086	rBV	634381	556158	9.10%	1.779%
22	15.394	1205	1208	1210	rBV	460670	531396	8.70%	1.699%

Sum of corrected areas: 31269012

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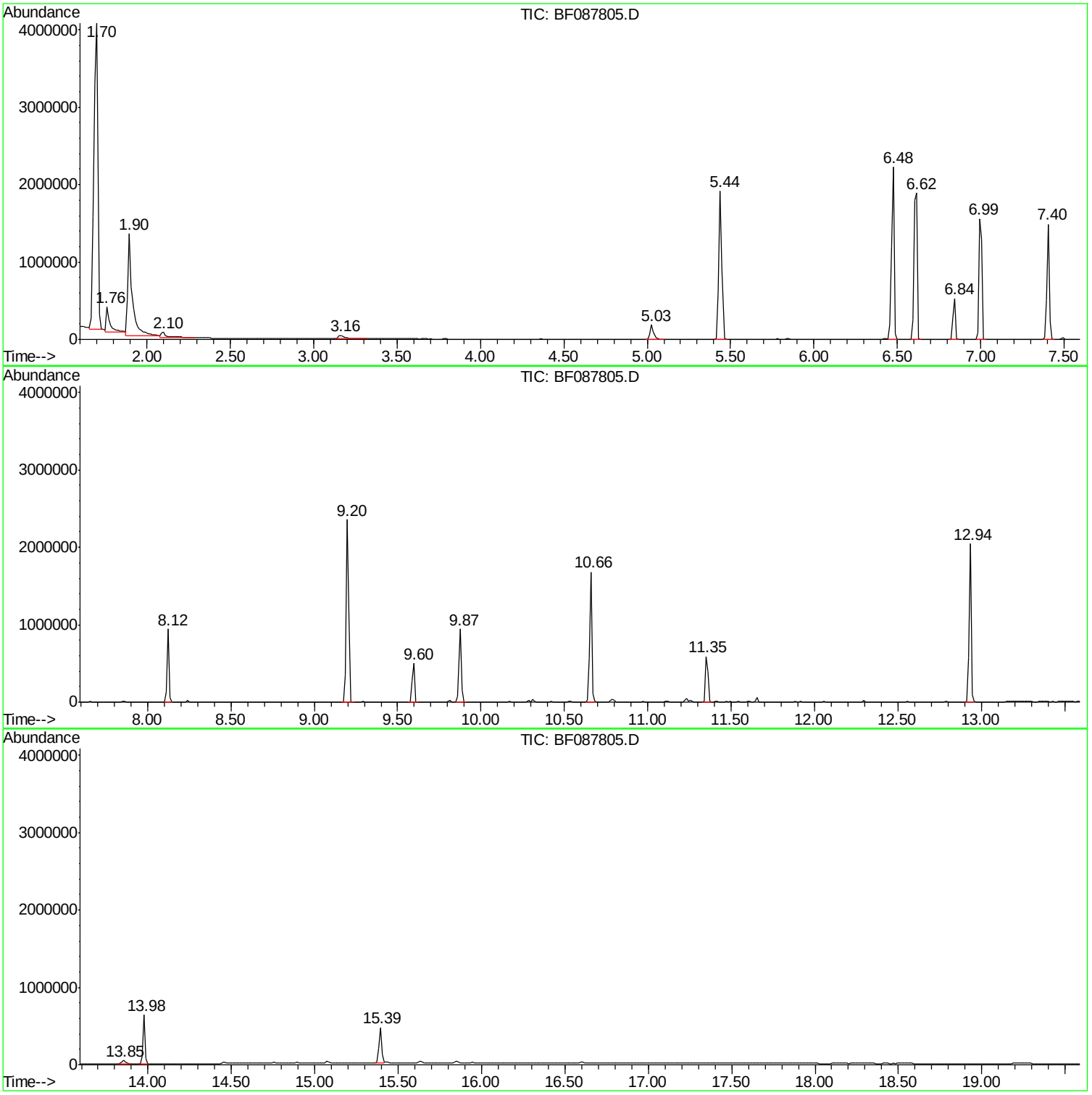
Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087804.D
Acq On : 8 Jun 2016 00:17
Operator : UM/SJ
Sample : H3379-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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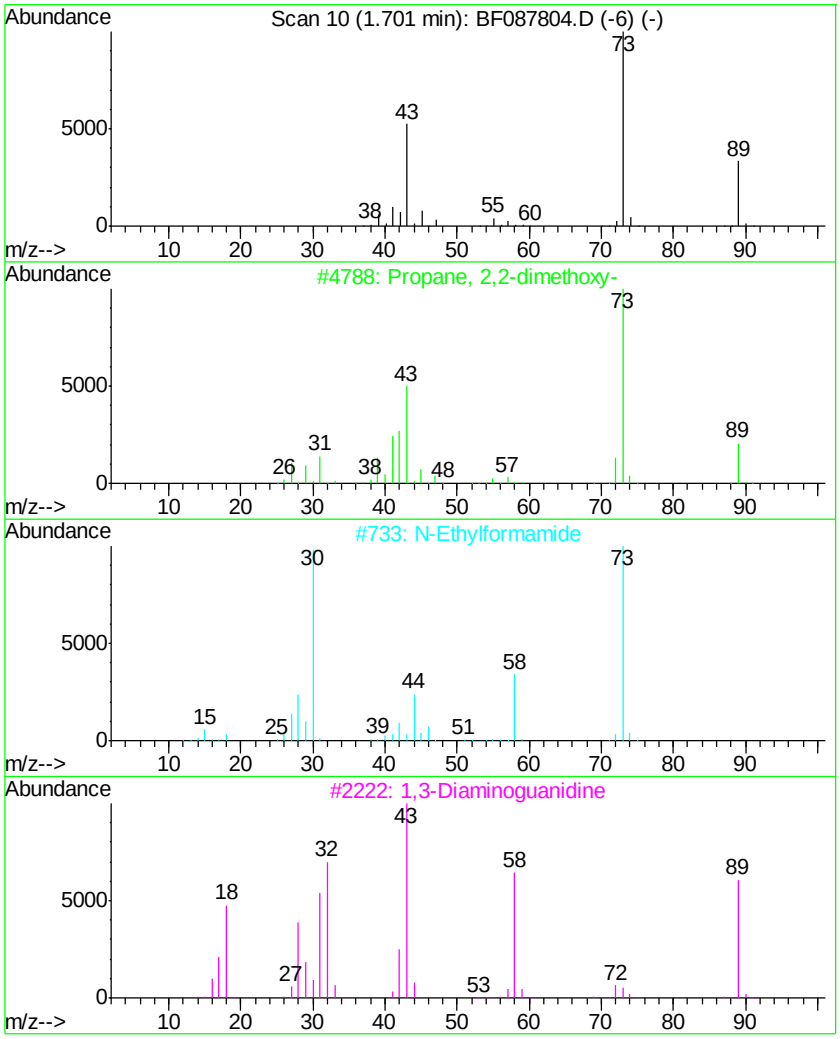
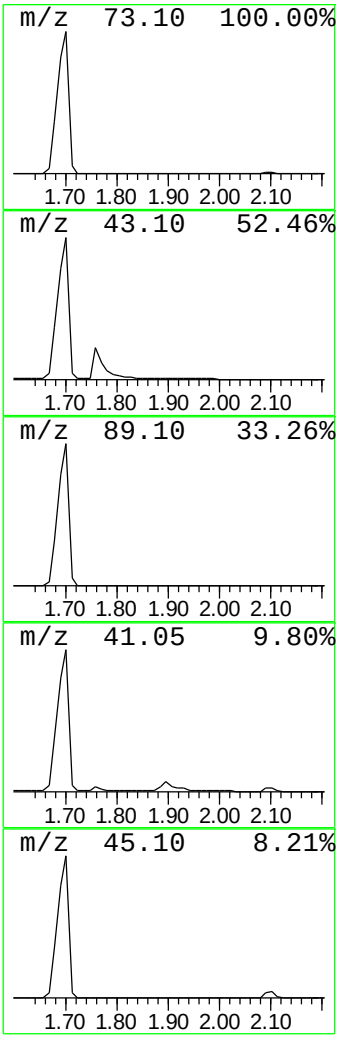
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	216.05 ng	6108610	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Operator : UM/SJ
Sample : H3379-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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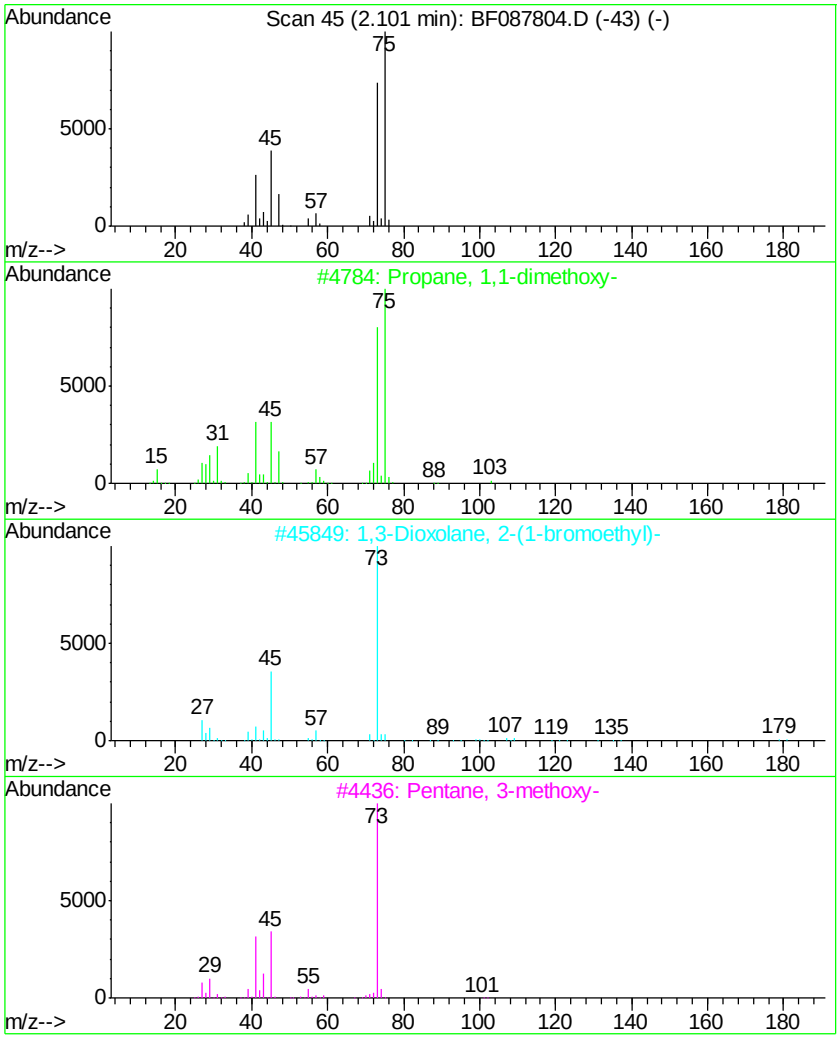
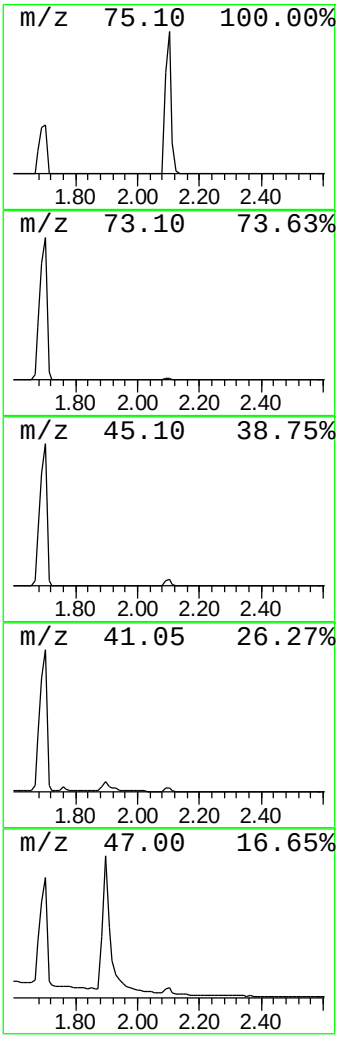
Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	6.73 ng	190171	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	17
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4	Glycine	75	C2H5NO2	000056-40-6	9
5	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060716\
Data File : BF087804.D
Acq On : 8 Jun 2016 00:17
Operator : UM/SJ
Sample : H3379-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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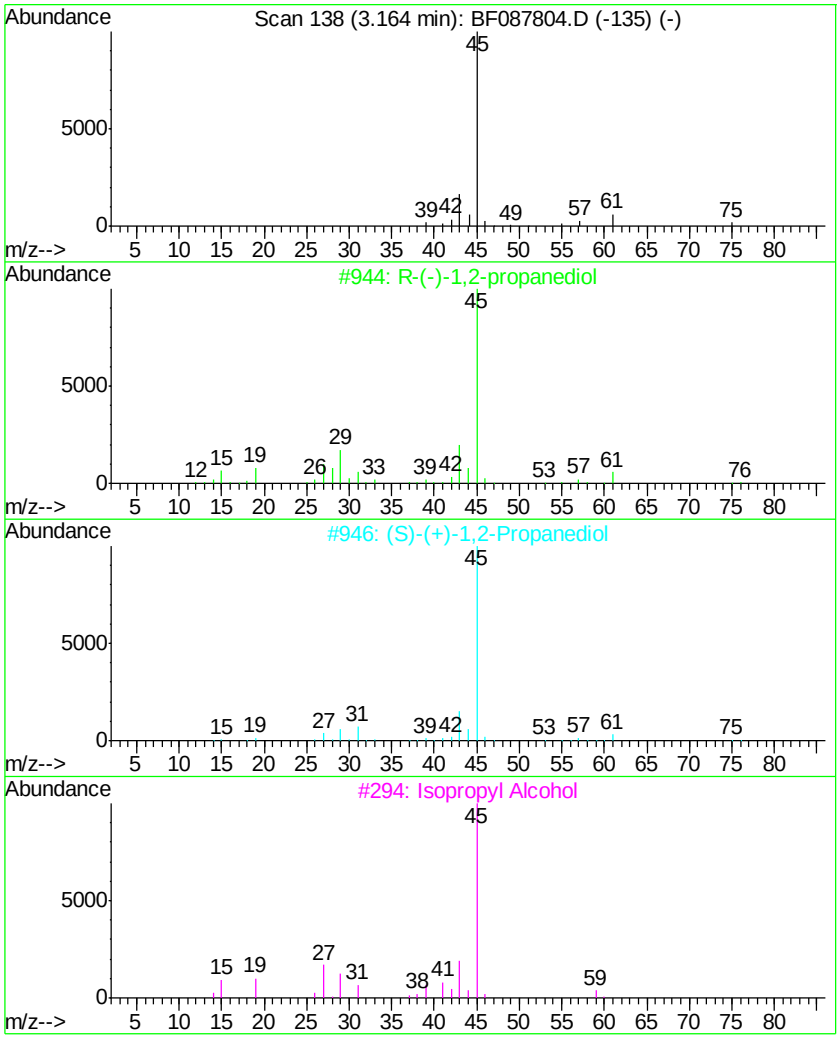
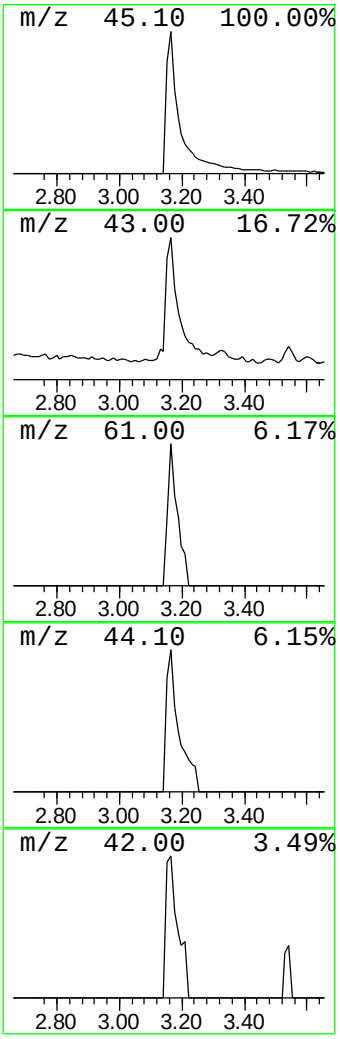
Peak Number 5 unknown3.16 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	3.48 ng	98279	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9





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Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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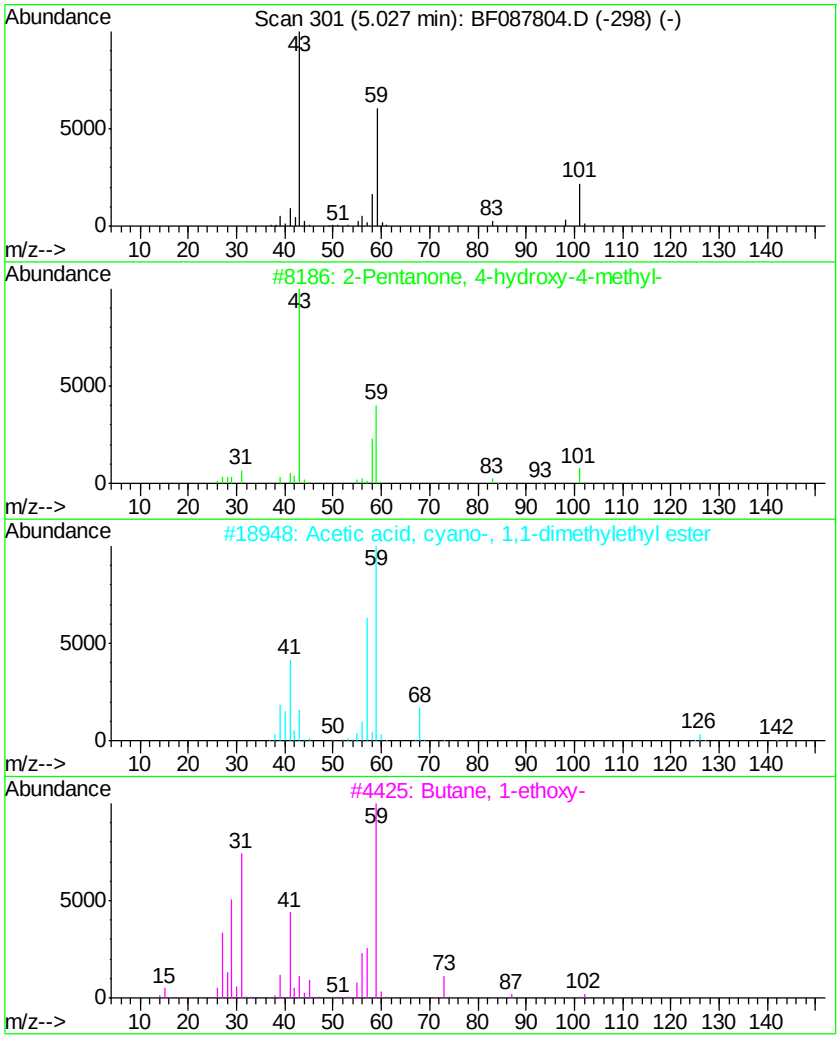
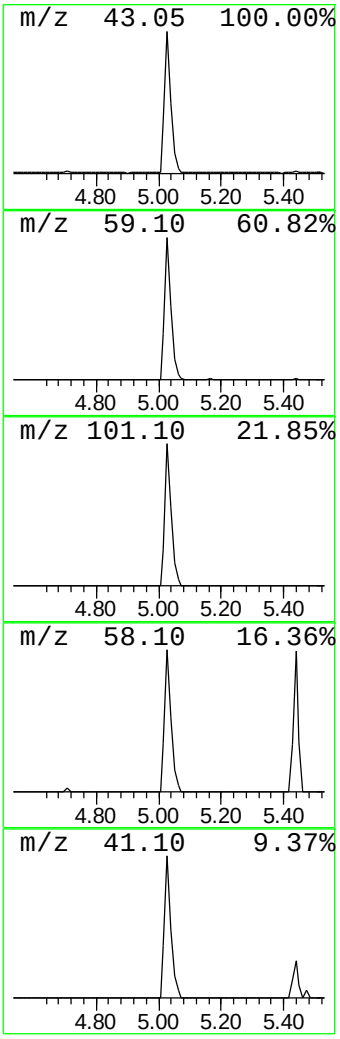
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	9.10 ng	257431	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : H3379-10
Misc :
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Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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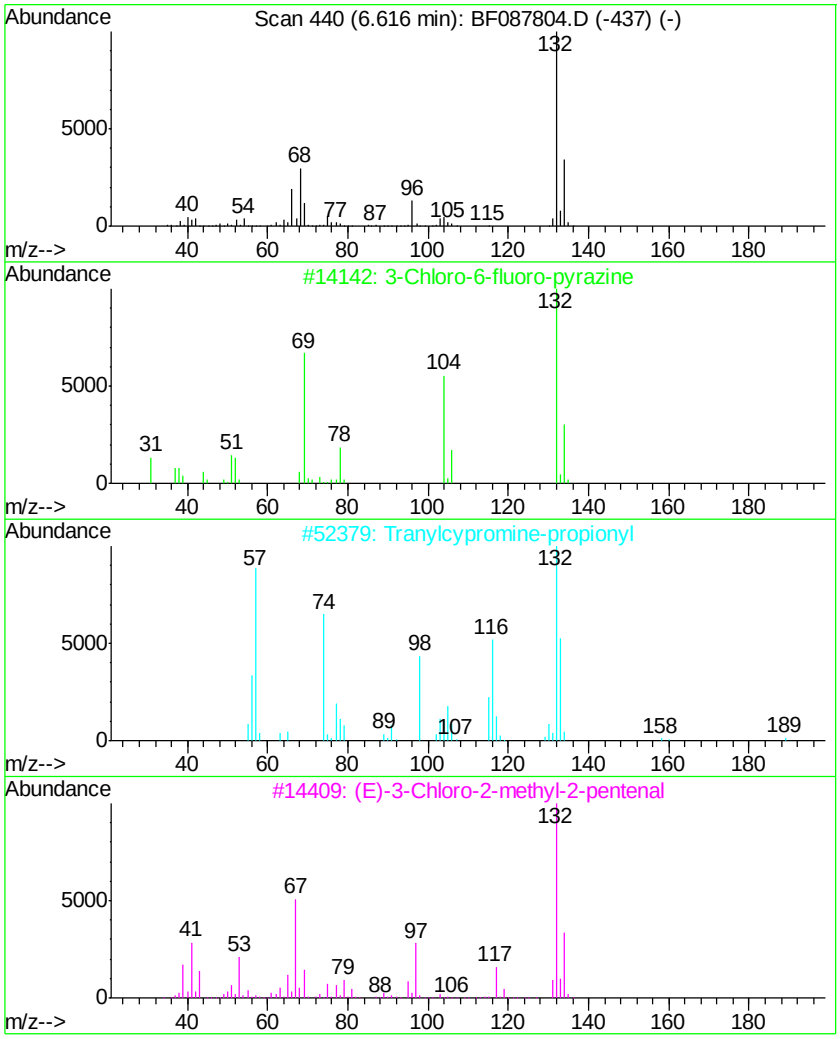
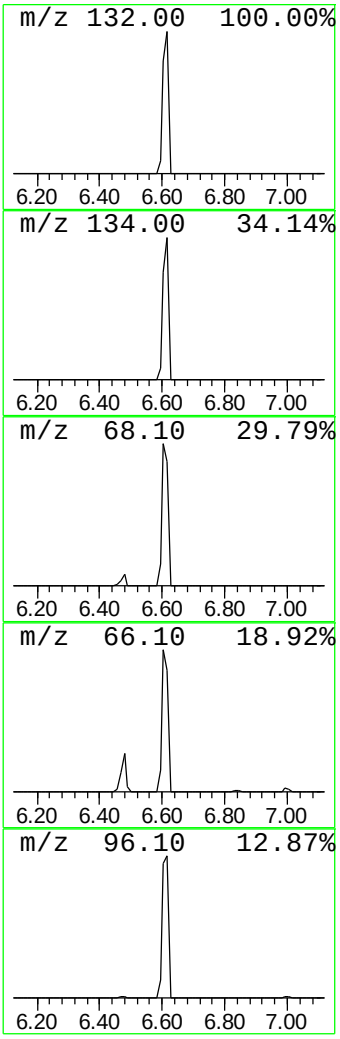
Peak Number 7 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.48 ng	2699760	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	52
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	37
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	33
4	Amphetaminil	250	C17H18N2	017590-01-1	28
5	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	25





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Sample : H3379-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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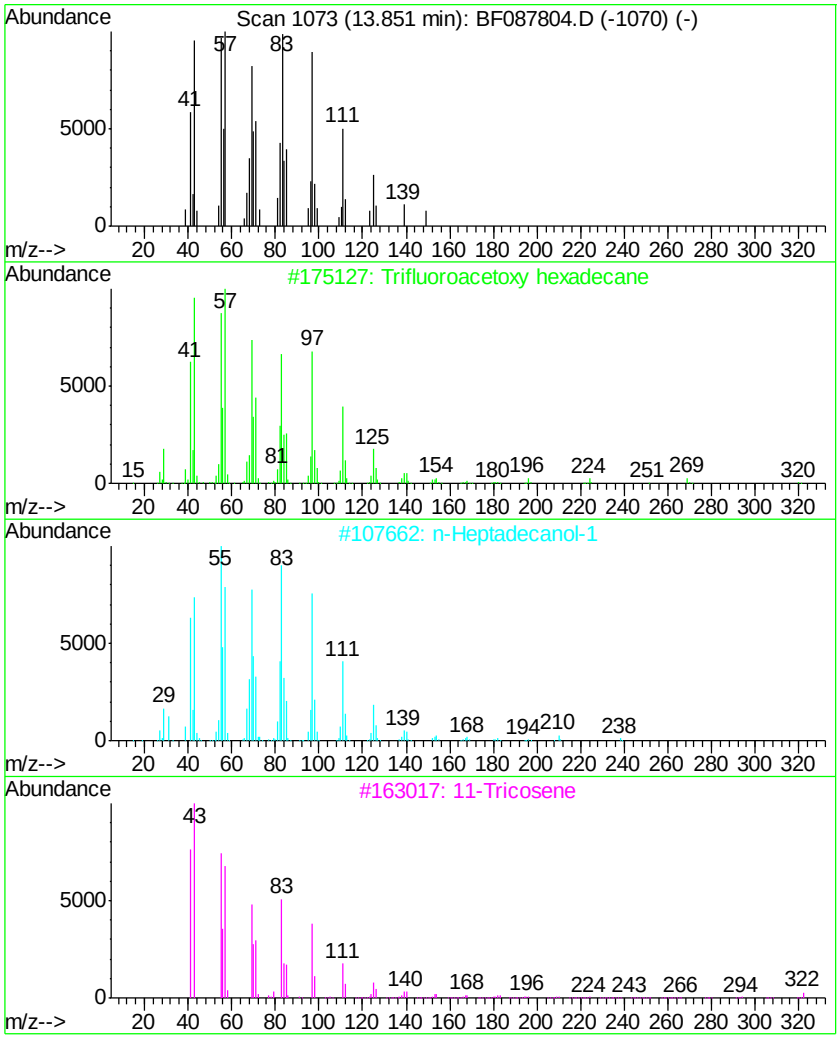
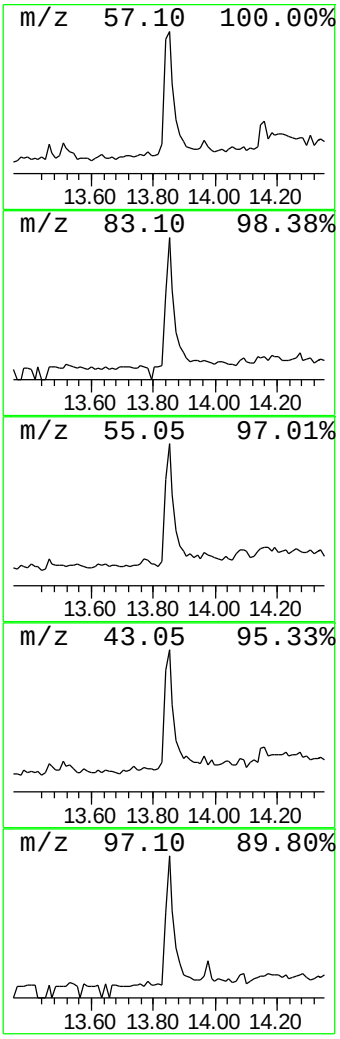
Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.28 ng	91325	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
3	11-Tricosene	322	C23H46	052078-56-5	87
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	86





Tentatively Identified Compound (LSC) summary

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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
Propane, 2,2-dime...	1.70	216.1	ng	6108610	1	6.84	565487	20.0
Propane, 1,1-dime...	2.10	6.7	ng	190171	1	6.84	565487	20.0
unknown3.16	3.16	3.5	ng	98279	1	6.84	565487	20.0
2-Pentanone, 4-hy...	5.03	9.1	ng	257431	1	6.84	565487	20.0
3-Chloro-6-fluoro...	6.62	95.5	ng	2699760	1	6.84	565487	20.0
Trifluoroacetoxy ...	13.85	3.3	ng	91325	5	13.98	556158	20.0