LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-06-6.0-16.0

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-BF072016.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	1.713	9	11	40	rVB	638124	1264870	70.65%	10.097%
2	2.296	59	62	65	rVB	21734	33198	1.85%	0.265%
3	4.696	270	272	283	rVB	71980	119415	6.67%	0.953%
4	5.153	310	312	334	rBV	447252	826150	46.15%	6.595%
5	6.227	405	406	414	rBV	409363	675076	37.71%	5.389%
6	6.342	414	416	431	rVV	868810	1140697	63.72%	9.106%
7	6.582	435	437	444	rBV	183993	262578	14.67%	2.096%
8	6.730	448	450	460	rVB	999650	1023257	57.16%	8.168%
9	7.153	484	487	496	rBV	690709	949723	53.05%	7.581%
10	7.862	547	549	560	rBV	379277	398284	22.25%	3.179%
11	8.948	641	644	646	rBV	1459361	1790238	100.00%	14.291%
12	9.336	676	678	684	rBV	43804	58156	3.25%	0.464%
13	9.611	699	702	704	rBV	407415	445038	24.86%	3.553%
14	10.399	768	771	773	rBV	646138	865370	48.34%	6.908%
15	10.971	819	821	827	rBV	21603	31673	1.77%	0.253%
16	11.085	828	831	835	rBV	387013	438897	24.52%	3.504%
17	11.394	856	858	861	rVB	14612	18590	1.04%	0.148%
18	12.502	953	955	958	rBV	53483	60246	3.37%	0.481%
19	12.662	967	969	972	rBV	1095617	1442582	80.58%	11.516%
20	13.211	1015	1017	1019	rBV	36237	38215	2.13%	0.305%
21	13.588	1047	1050	1058	rVB	13967	28247	1.58%	0.225%
22	13.702	1058	1060	1068	rBV	349293	365935	20.44%	2.921%
23	15.040	1175	1177	1181	rBV	184516	250435	13.99%	1.999%

Sum of corrected areas: 12526870

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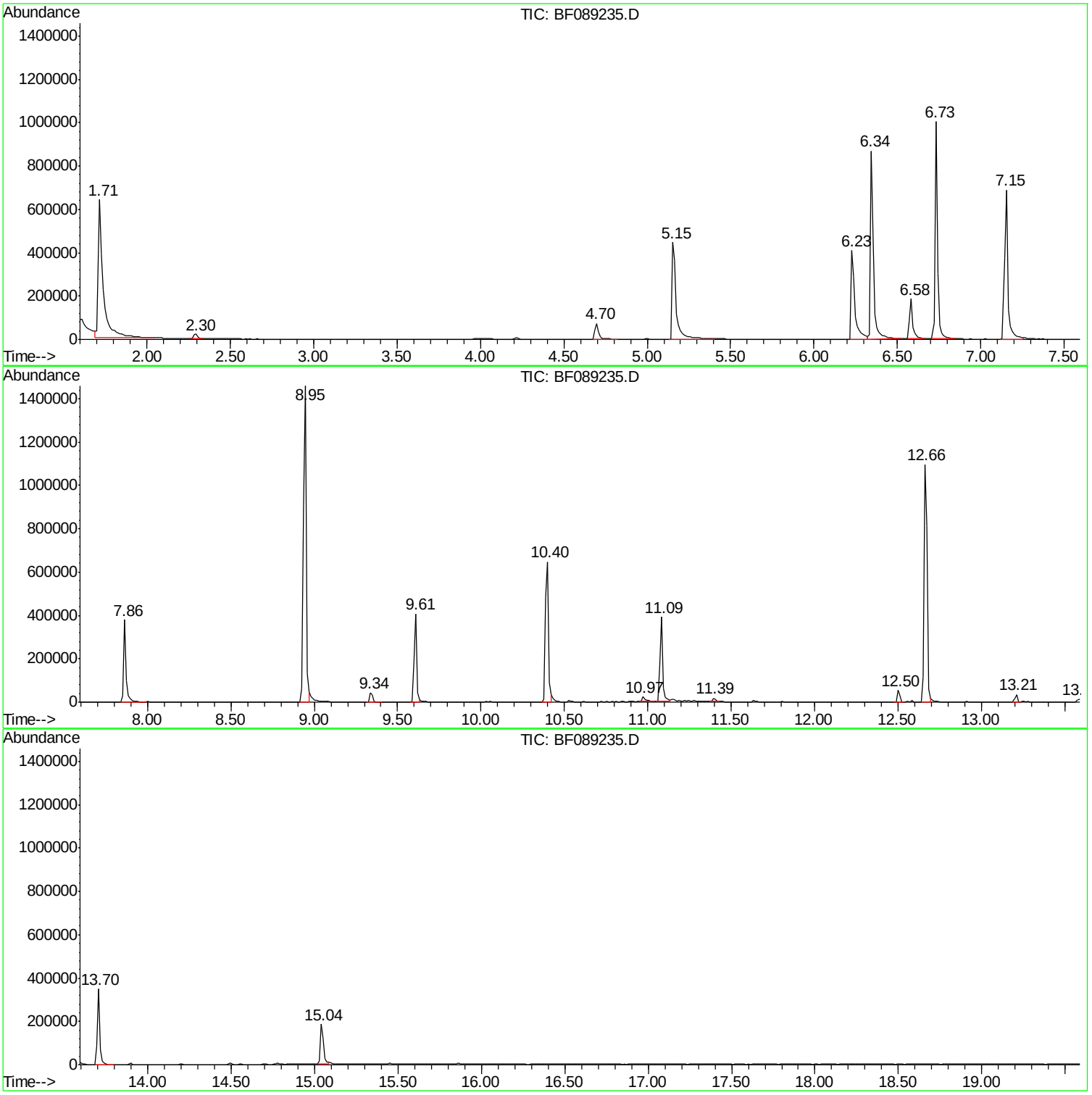
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-06-6.0-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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 : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
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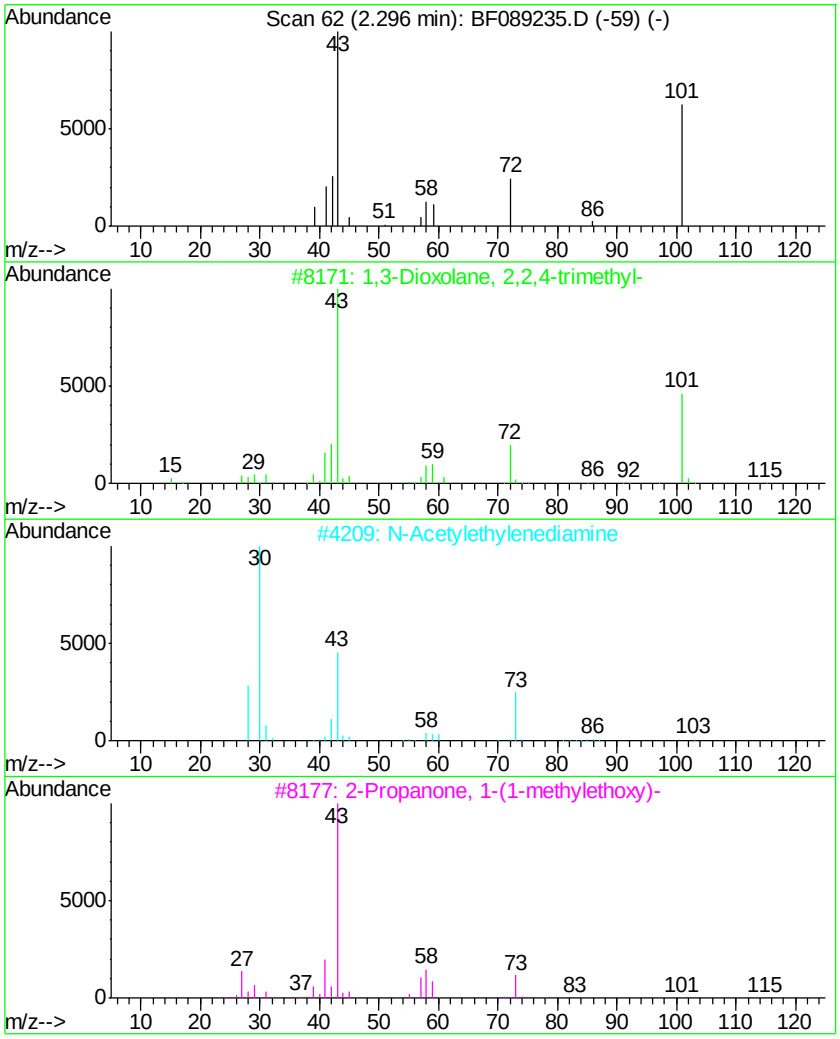
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

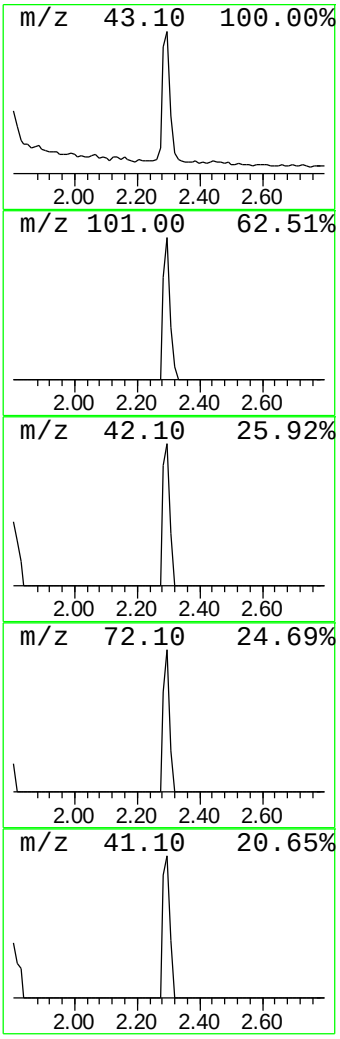
****

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	2.53 ng	33198	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	9
3	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	7
5	Butane	58	C4H10	000106-97-8	7





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-06-6.0-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

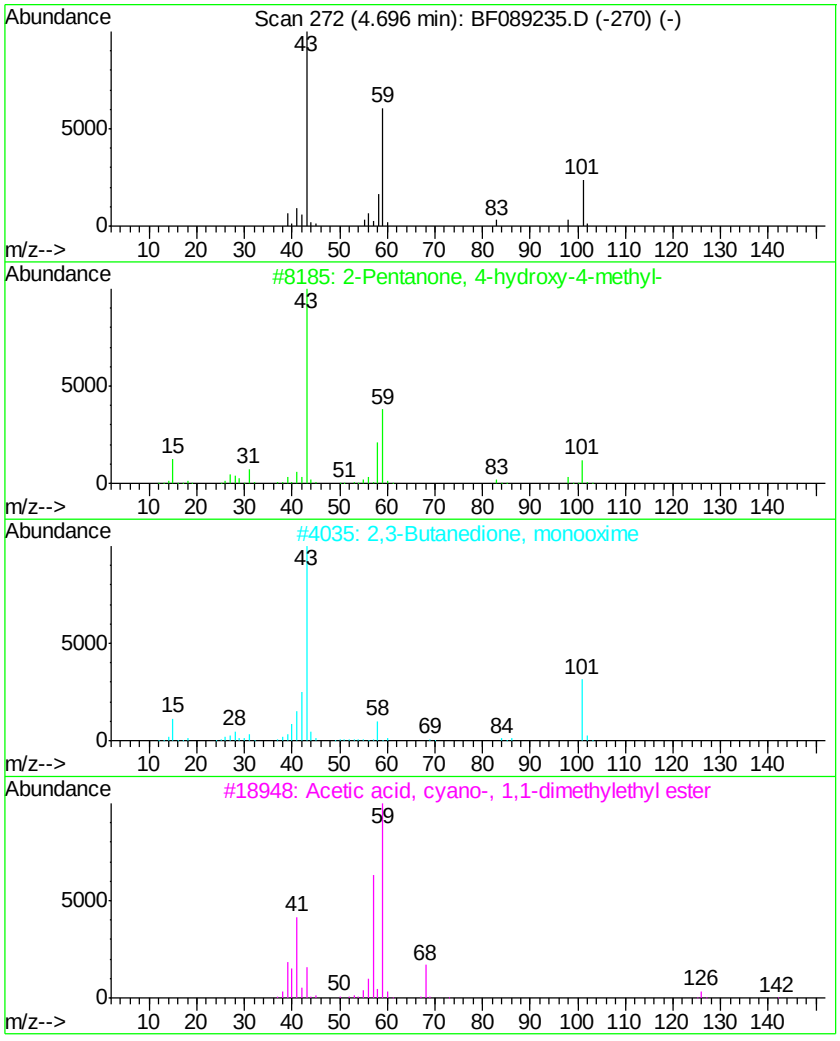
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

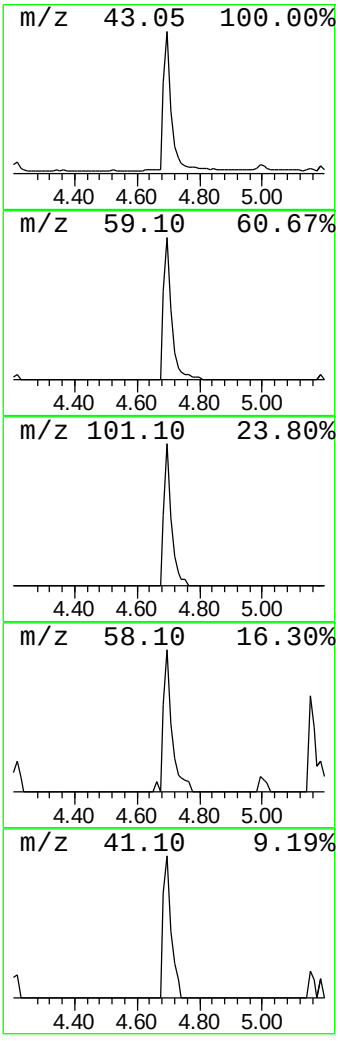
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	9.10 ng	119415	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	Acetone	58	C3H6O	000067-64-1	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-06-6.0-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

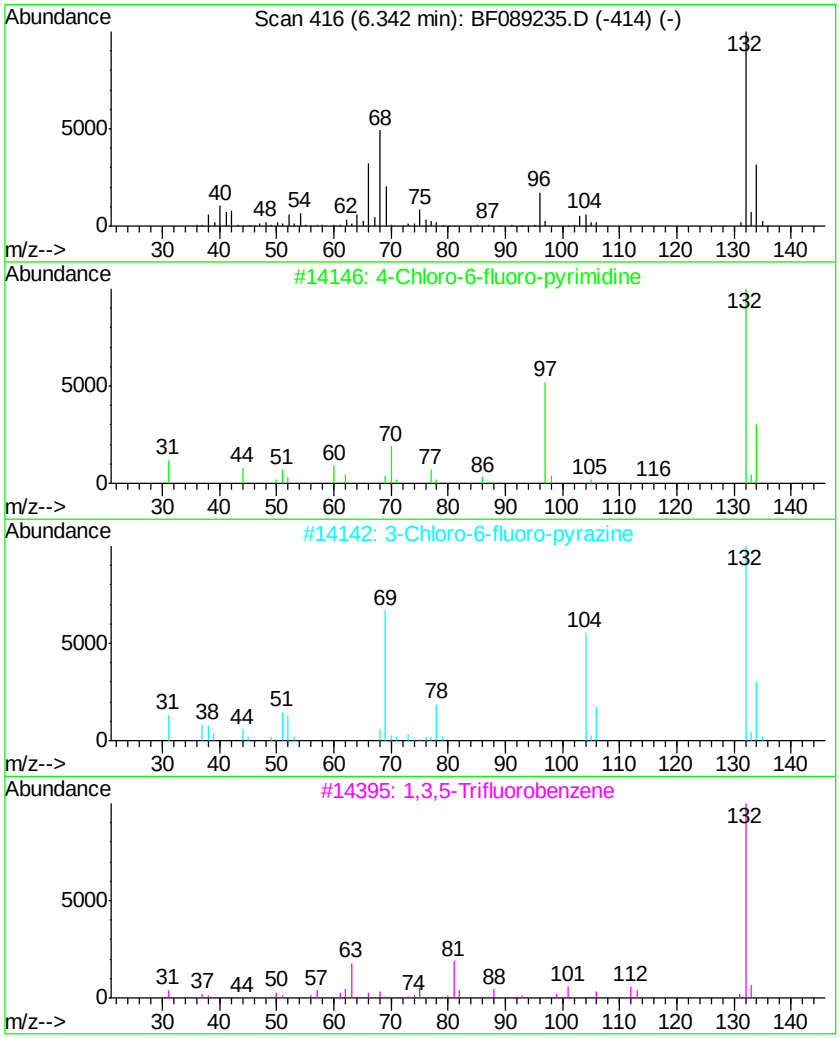
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

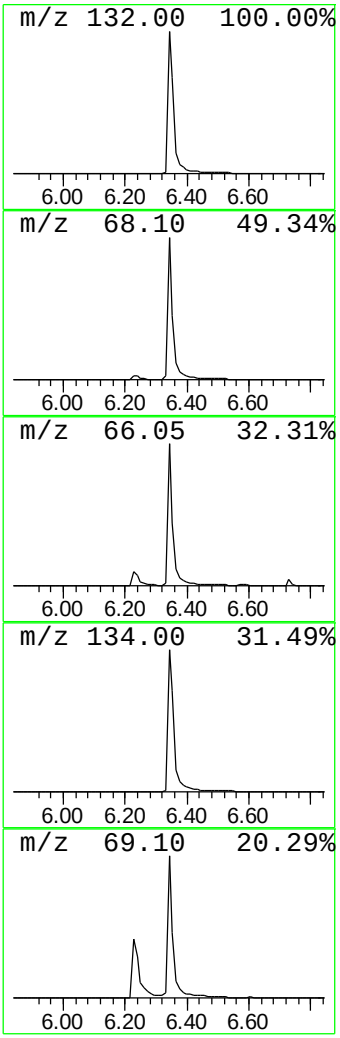
****

Peak Number 4 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	86.88 ng	1140700	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Data File : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-06-6.0-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

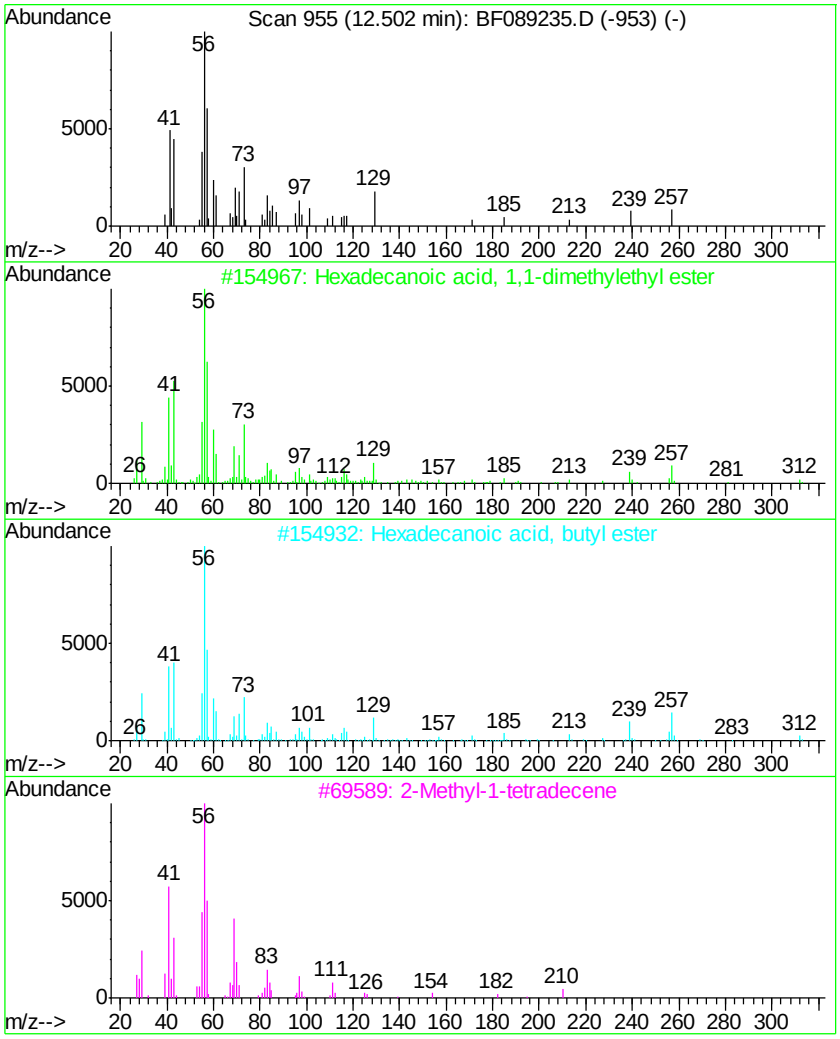
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

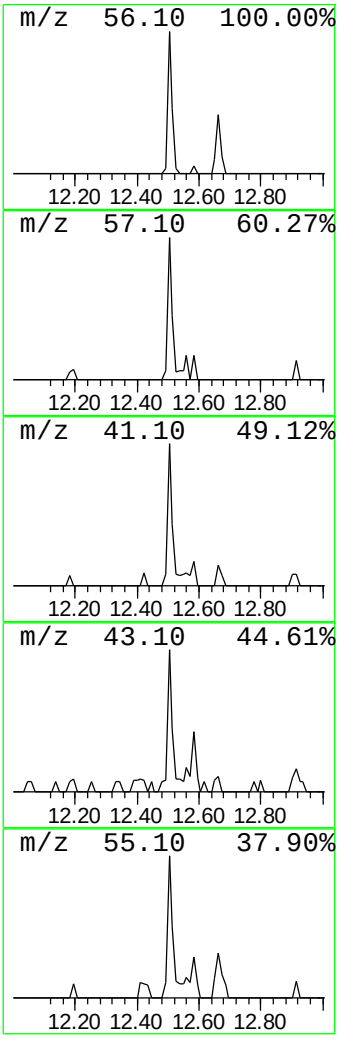
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	3.29 ng	60246	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3	2-Methyl-1-tetradecene	210	C15H30	052254-38-3	38
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089235.D
Acq On : 23 Jul 2016 14:01
Operator : UM/SJ
Sample : H4120-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-06-6.0-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

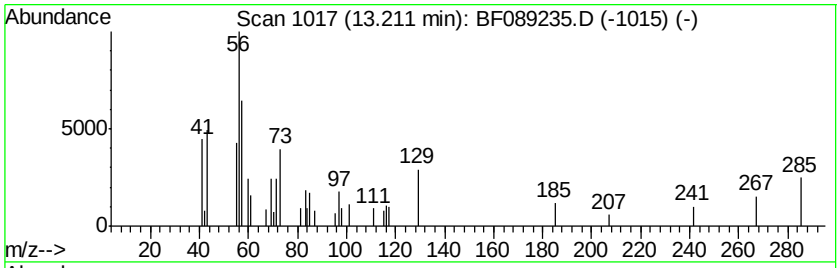
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

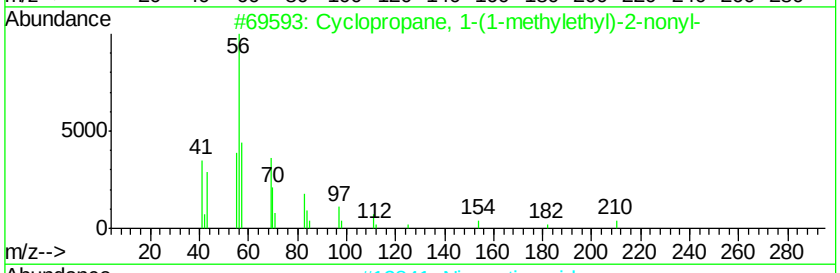
****

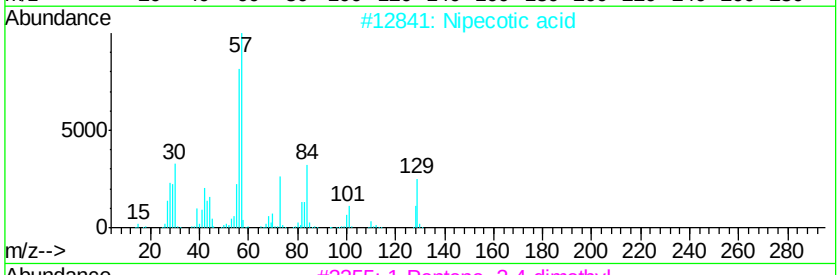
Peak Number 7 unknown13.21 Concentration Rank 7

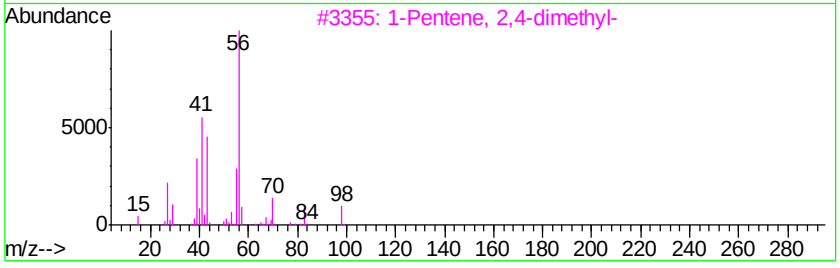
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.09 ng	38215	Chrysene-d12	13.70

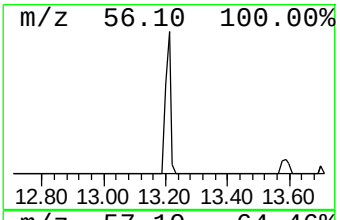
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
2	Nipecotic acid	129	C6H11NO2	000498-95-3	32
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	25
5	2-Methylhexadec-1-ene	238	C17H34	061868-19-7	25

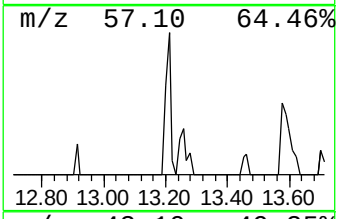


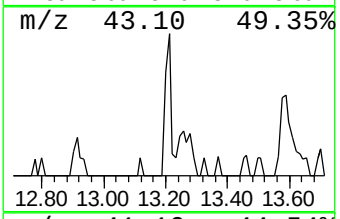


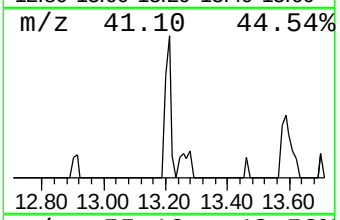


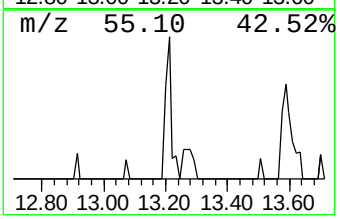












Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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
1,3-Dioxolane, 2,...	2.30	2.5	ng	33198	1	6.58	262578	20.0
2-Pentanone, 4-hy...	4.70	9.1	ng	119415	1	6.58	262578	20.0
unknown6.34	6.34	86.9	ng	1140700	1	6.58	262578	20.0
Hexadecanoic acid...	12.50	3.3	ng	60246	5	13.70	365935	20.0
unknown13.21	13.21	2.1	ng	38215	5	13.70	365935	20.0