LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.690	7	9	18	rVB	318469	586349	23.85%	2.509%
2	1.815	18	20	32	rVV	1449332	2458741	100.00%	10.519%
3	1.964	32	33	43	rVB	47893	117467	4.78%	0.503%
4	4.913	288	291	300	rBV	148019	232126	9.44%	0.993%
5	5.336	325	328	331	rBV	1892857	1912977	77.80%	8.184%
6	6.387	417	420	422	rBV	1919770	2203842	89.63%	9.429%
7	6.513	428	431	433	rBV	1948238	2222611	90.40%	9.509%
8	6.742	449	451	453	rBV	724968	598554	24.34%	2.561%
9	6.902	462	465	467	rBV	1650495	1818981	73.98%	7.782%
10	7.313	498	501	503	rBV	1362680	1494785	60.79%	6.395%
11	8.033	561	564	566	rBV	630520	756029	30.75%	3.235%
12	9.108	655	658	661	rBV	2404458	2253689	91.66%	9.642%
13	9.508	691	693	695	rBV	320862	319235	12.98%	1.366%
14	9.782	714	717	719	rVB	932552	842293	34.26%	3.604%
15	10.216	754	755	757	rVB	39328	39492	1.61%	0.169%
16	10.571	783	786	788	rBV	1113312	1239386	50.41%	5.303%
17	10.696	795	797	803	rBV	42637	63929	2.60%	0.274%
18	11.142	834	836	837	rBV	30565	32635	1.33%	0.140%
19	11.256	844	846	849	rBV	730780	689708	28.05%	2.951%
20	12.845	982	985	988	rBV	1852912	1730858	70.40%	7.405%
21	13.337	1024	1028	1030	rBV	408657	591120	24.04%	2.529%
22	13.760	1062	1065	1074	rBV2	18045	56706	2.31%	0.243%
23	13.885	1074	1076	1079	rVV	425704	553306	22.50%	2.367%
24	15.291	1196	1199	1202	rBV	422153	558410	22.71%	2.389%

Sum of corrected areas: 23373229

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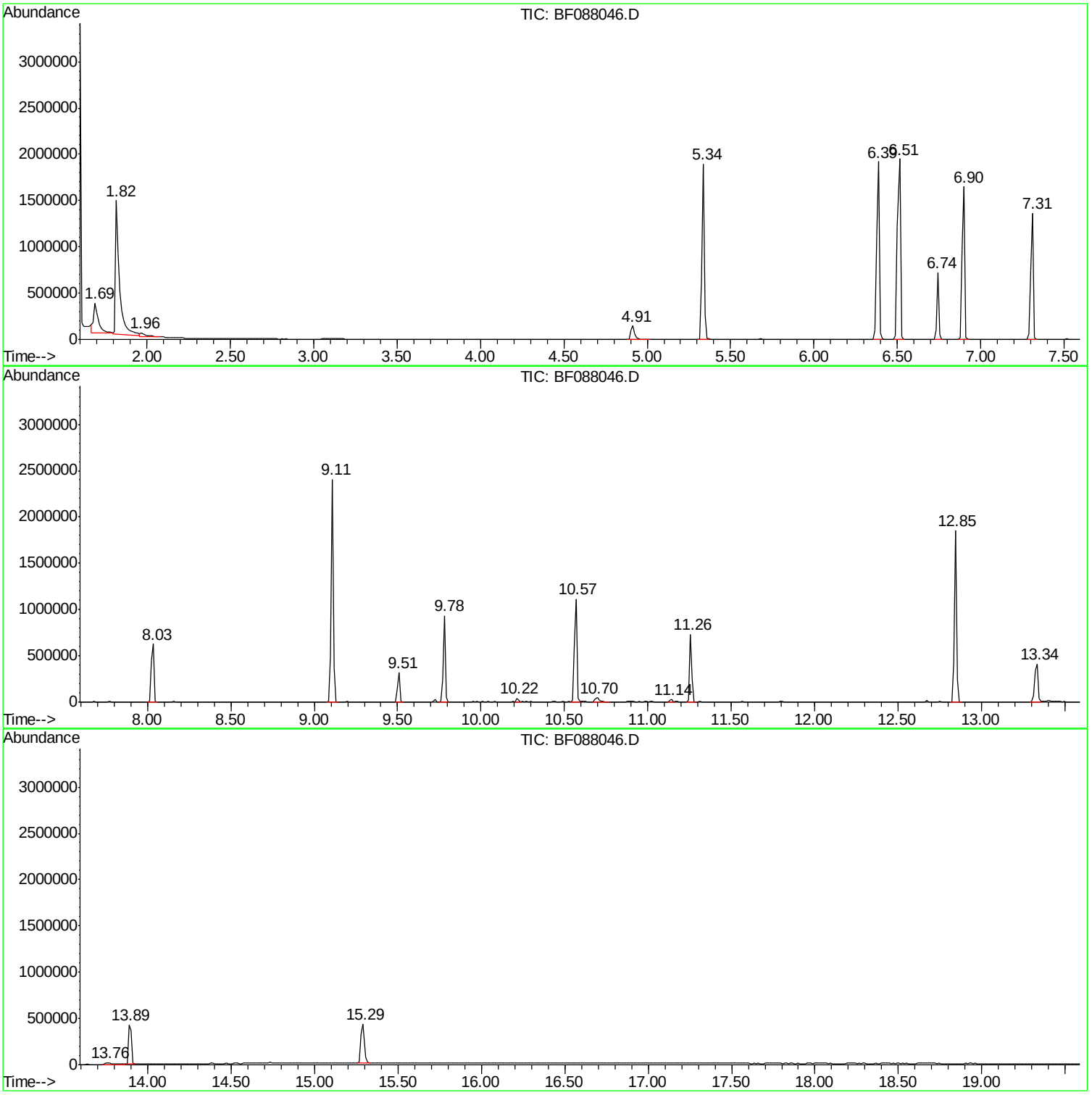
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
181-05-EB-06142016

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\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
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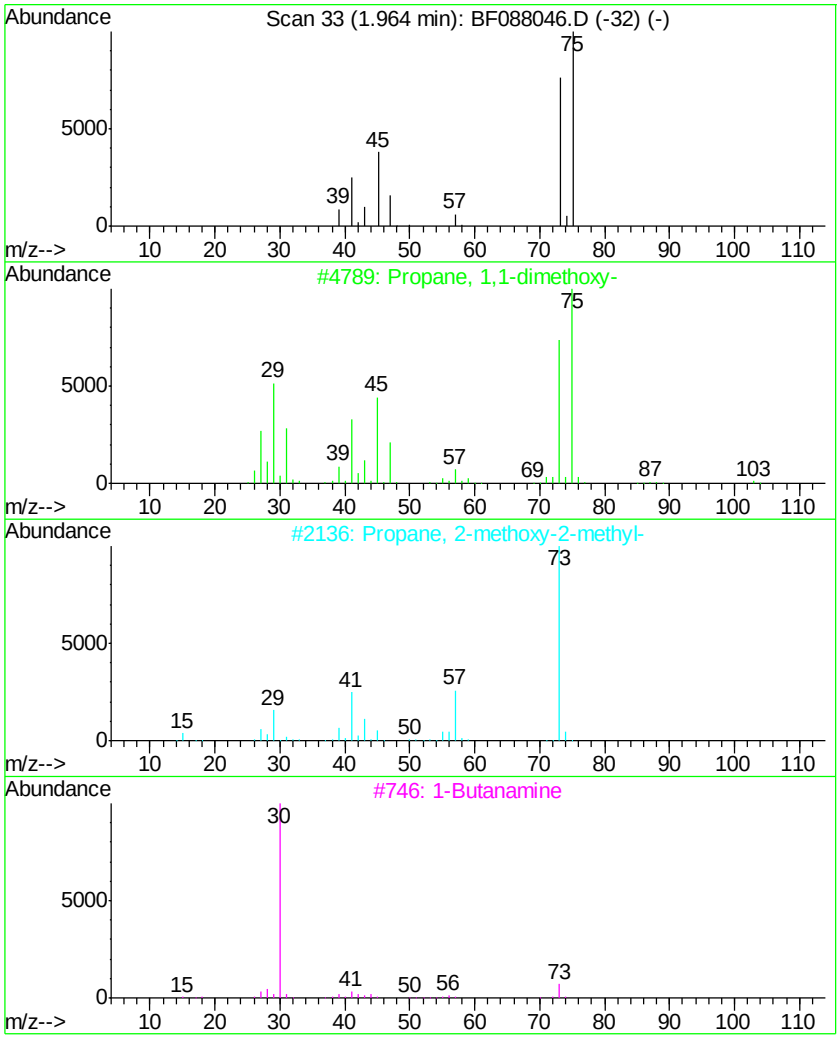
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

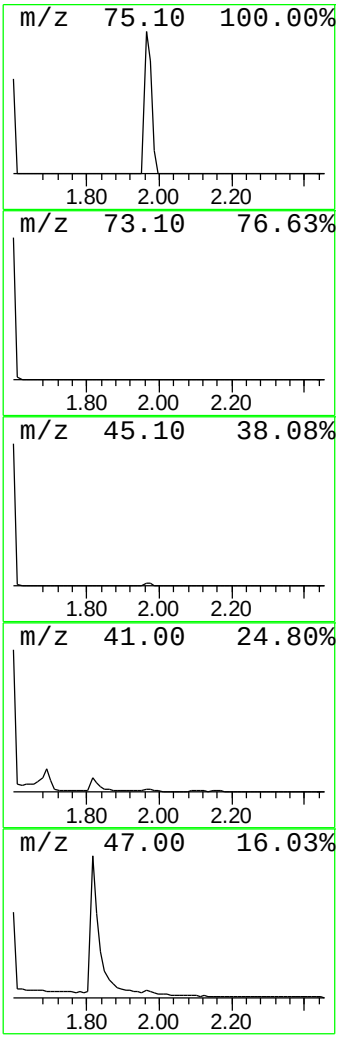
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	3.93 ng	117467	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Glycine	75	C2H5NO2	000056-40-6	4
5	N-Ethylformamide	73	C3H7NO	000627-45-2	4





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Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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

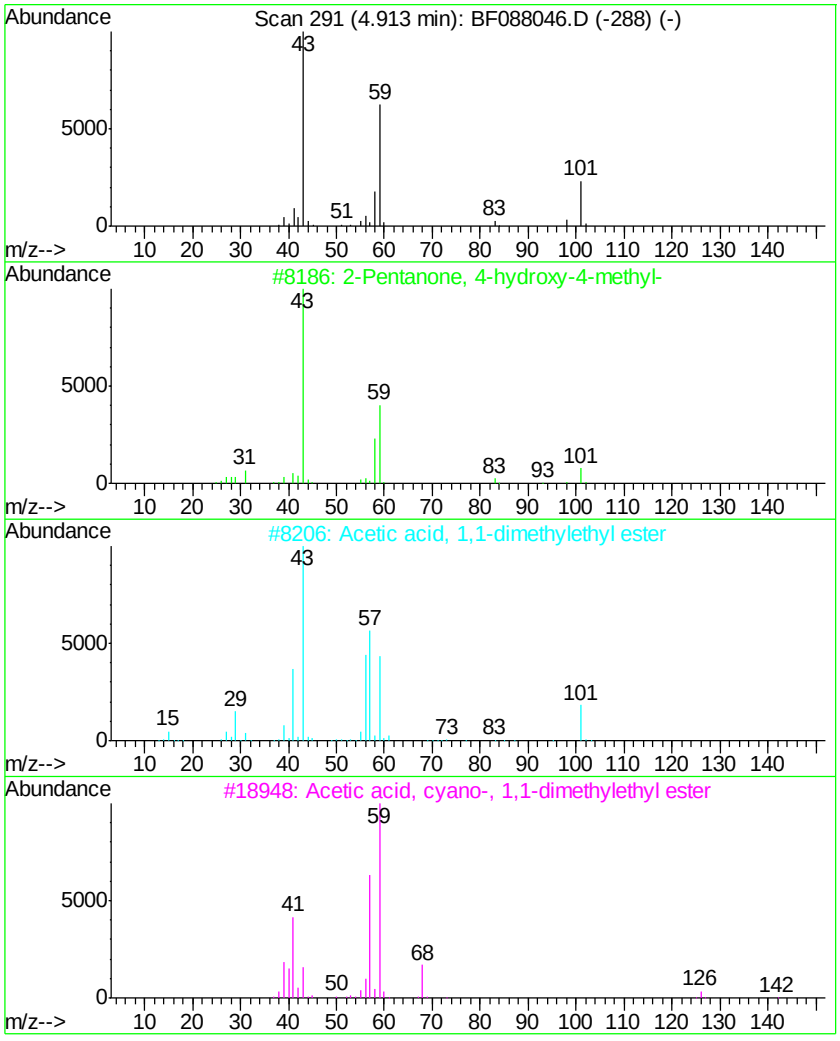
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

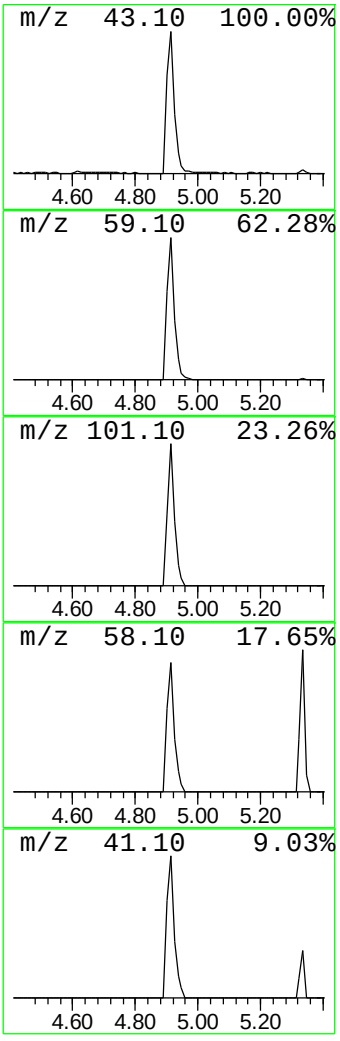
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	7.76 ng	232126	1,4-Dichlorobenzene-d4	6.74

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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

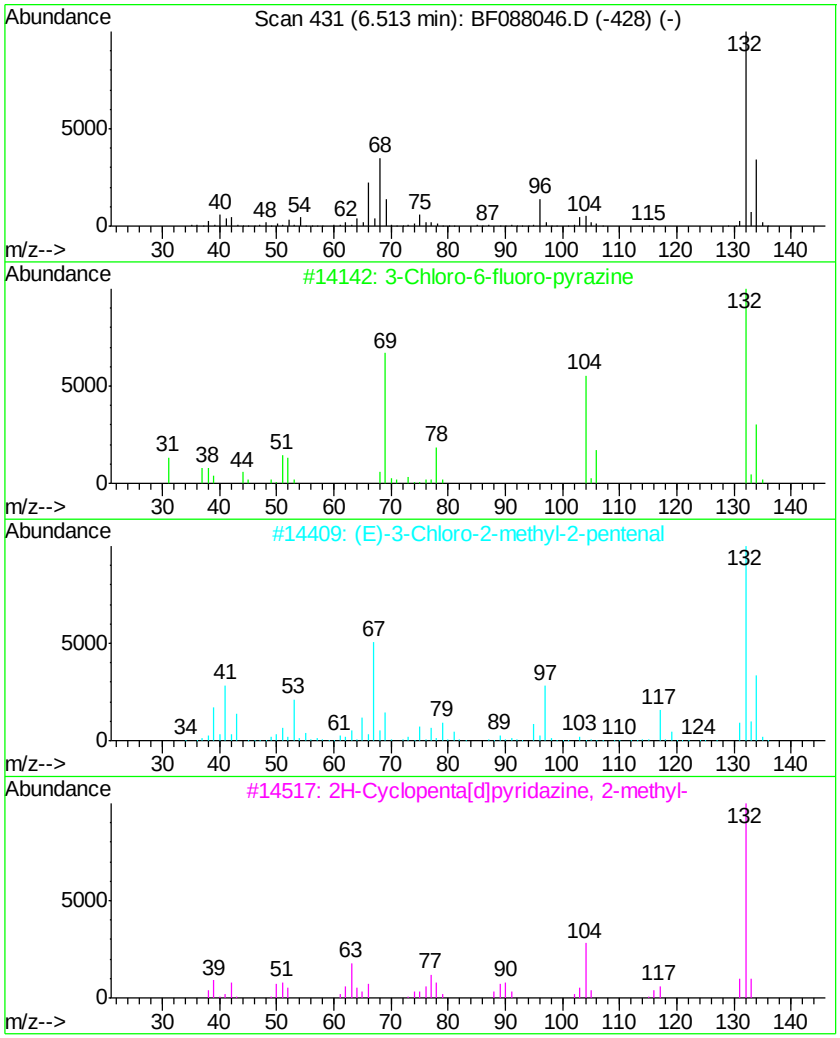
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

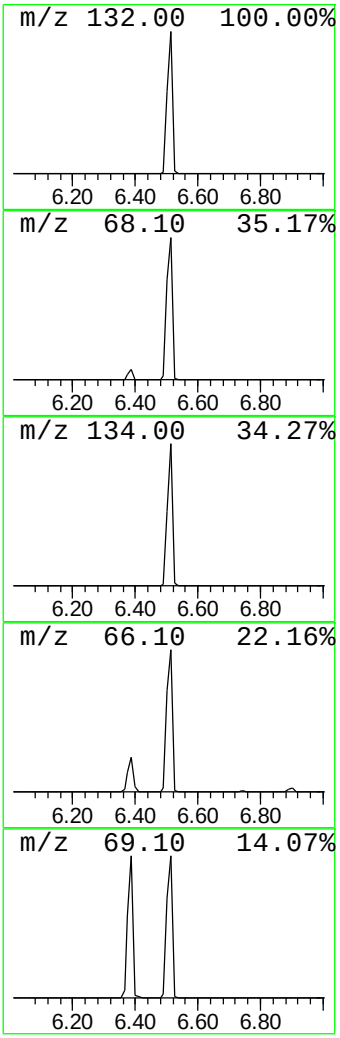
****

Peak Number 5 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	74.27 ng	2222610	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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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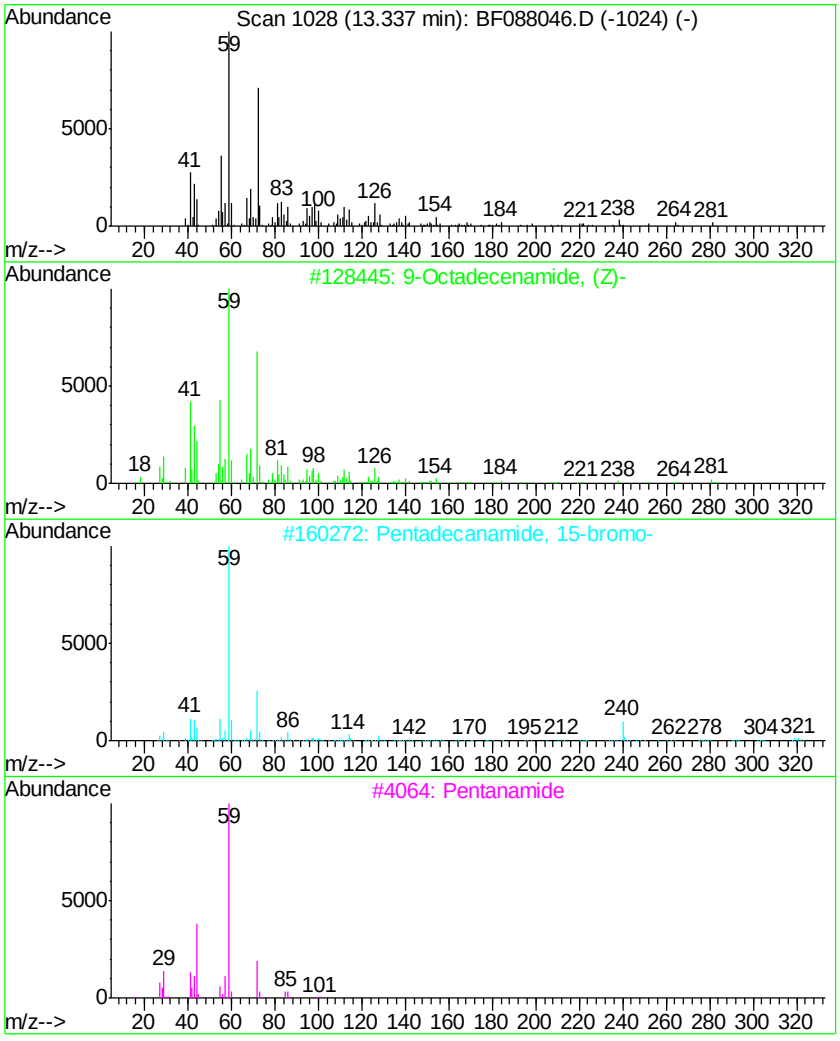
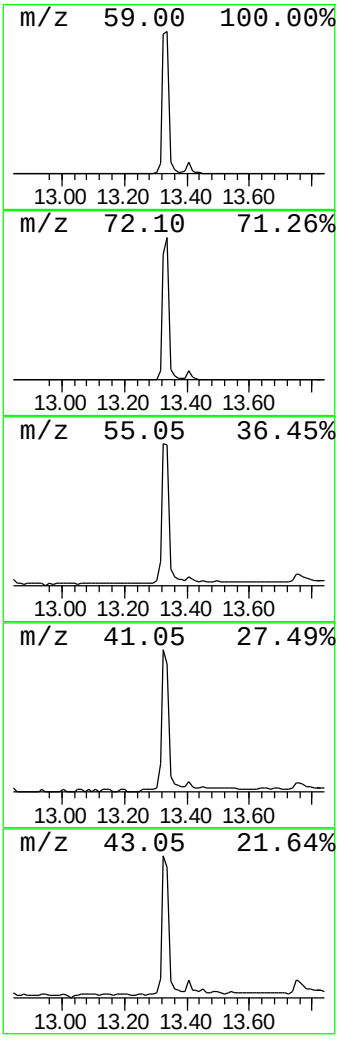
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	21.37 ng	591120	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
3	Pentanamide	101	C5H11NO	000626-97-1	50
4	Dodecanamide	199	C12H25NO	001120-16-7	50
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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

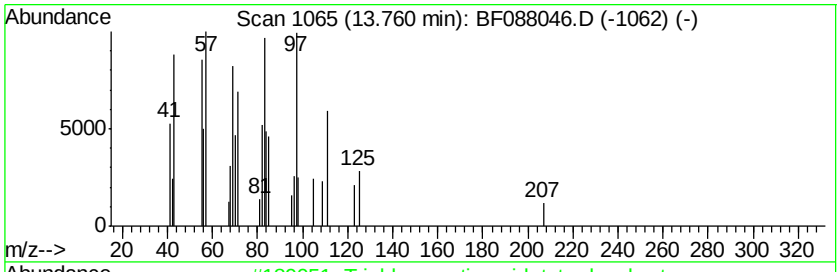
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

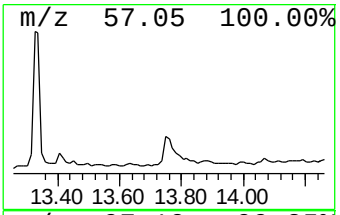
****

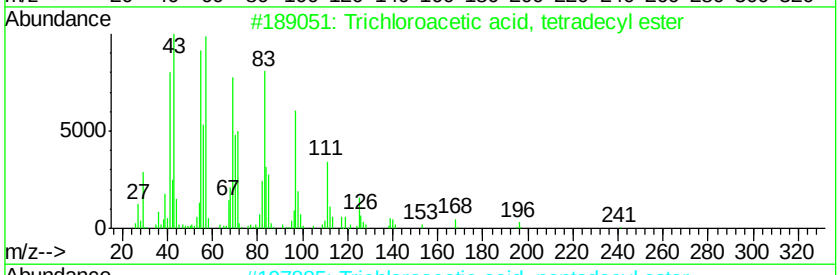
Peak Number 8 Trichloroacetic acid, tetra... Concentration Rank 8

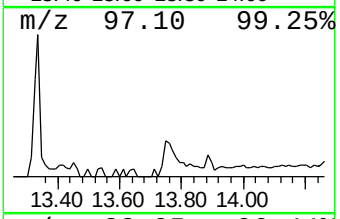
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	2.05 ng	56706	Chrysene-d12	13.90

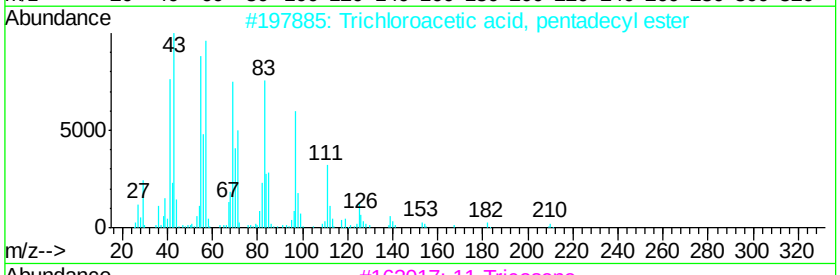
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	11-Tricosene	322	C23H46	052078-56-5	87
4	1-Heptacosanol	396	C27H56O	002004-39-9	87
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	83

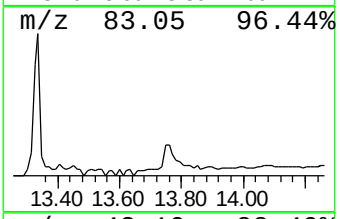


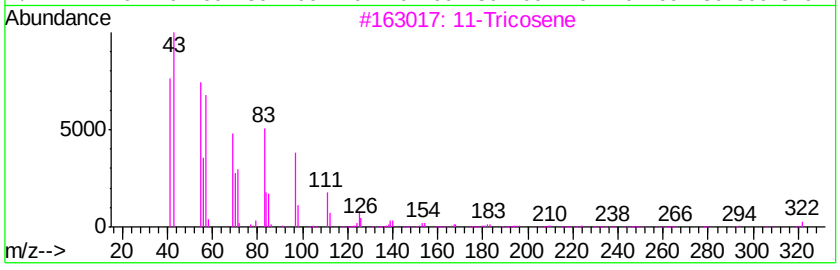


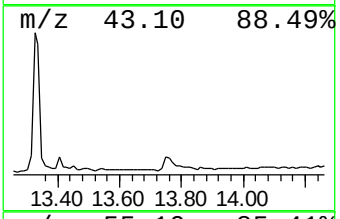


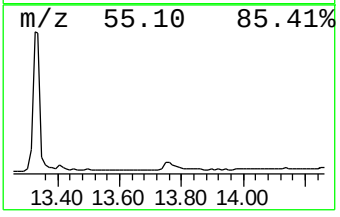












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
Data File : BF088046.D
Acq On : 15 Jun 2016 21:06
Operator : UM/SJ
Sample : H3609-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 181-05-EB-06142016

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.96	3.9	ng	117467	1	6.74	598554	20.0
2-Pentanone, 4-hy...	4.91	7.8	ng	232126	1	6.74	598554	20.0
unknown6.51	6.51	74.3	ng	2222610	1	6.74	598554	20.0
9-Octadecenamide,...	13.34	21.4	ng	591120	5	13.90	553306	20.0
Trichloroacetic a...	13.76	2.0	ng	56706	5	13.90	553306	20.0