LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

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-BF121716.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	4.270	189	191	195	rBV	224657	281610	3.50%	0.380%
2	4.944	247	250	260	rBV	2299423	4060270	50.46%	5.483%
3	5.378	285	288	290	rBV	7048714	8046297	100.00%	10.865%
4	5.436	290	293	301	rVB2	49685	90228	1.12%	0.122%
5	6.407	375	378	381	rBV	4814004	7855656	97.63%	10.607%
6	6.533	386	389	392	rBV	5775310	7003999	87.05%	9.457%
7	6.761	407	409	412	rBV	1733269	1676893	20.84%	2.264%
8	6.921	420	423	425	rBV	5142337	4777288	59.37%	6.451%
9	7.333	455	459	461	rBV	4284431	4914693	61.08%	6.636%
10	8.053	519	522	524	rBV	2231067	2426648	30.16%	3.277%
11	9.127	613	616	619	rBV	5500405	6389862	79.41%	8.628%
12	9.527	648	651	653	rBV	953776	1025244	12.74%	1.384%
13	9.802	672	675	677	rBV	2926039	2749638	34.17%	3.713%
14	10.248	712	714	715	rVB	126045	131959	1.64%	0.178%
15	10.465	730	733	736	rBV	64163	99131	1.23%	0.134%
16	10.590	741	744	747	rBV	4040960	4748542	59.02%	6.412%
17	10.716	753	755	760	rVB	249001	299299	3.72%	0.404%
18	11.162	792	794	796	rBV	275048	253140	3.15%	0.342%
19	11.288	802	805	807	rBV	2511629	2779545	34.54%	3.753%
20	11.585	829	831	834	rBV	210471	227734	2.83%	0.308%
21	11.733	842	844	847	rBV	162354	222216	2.76%	0.300%
22	11.825	850	852	856	rBV2	214529	241005	3.00%	0.325%
23	11.996	863	867	868	rBV2	81149	105059	1.31%	0.142%
24	12.202	882	885	887	rBV	155498	205339	2.55%	0.277%
25	12.876	941	944	946	rBV	5830813	6409997	79.66%	8.655%
26	13.768	1021	1022	1032	rVB	488879	687382	8.54%	0.928%
27	13.916	1032	1035	1037	rBV	2510507	2402912	29.86%	3.245%
28	14.408	1076	1078	1087	rVB	232628	312317	3.88%	0.422%
29	14.671	1099	1101	1107	rBV2	71343	135233	1.68%	0.183%
30	15.014	1128	1131	1132	rBV	54632	83764	1.04%	0.113%
31	15.322	1155	1158	1160	rBV	1409185	1874811	23.30%	2.532%
32	19.083	1481	1487	1497	rVB	470687	1540692	19.15%	2.080%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

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-BF121716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

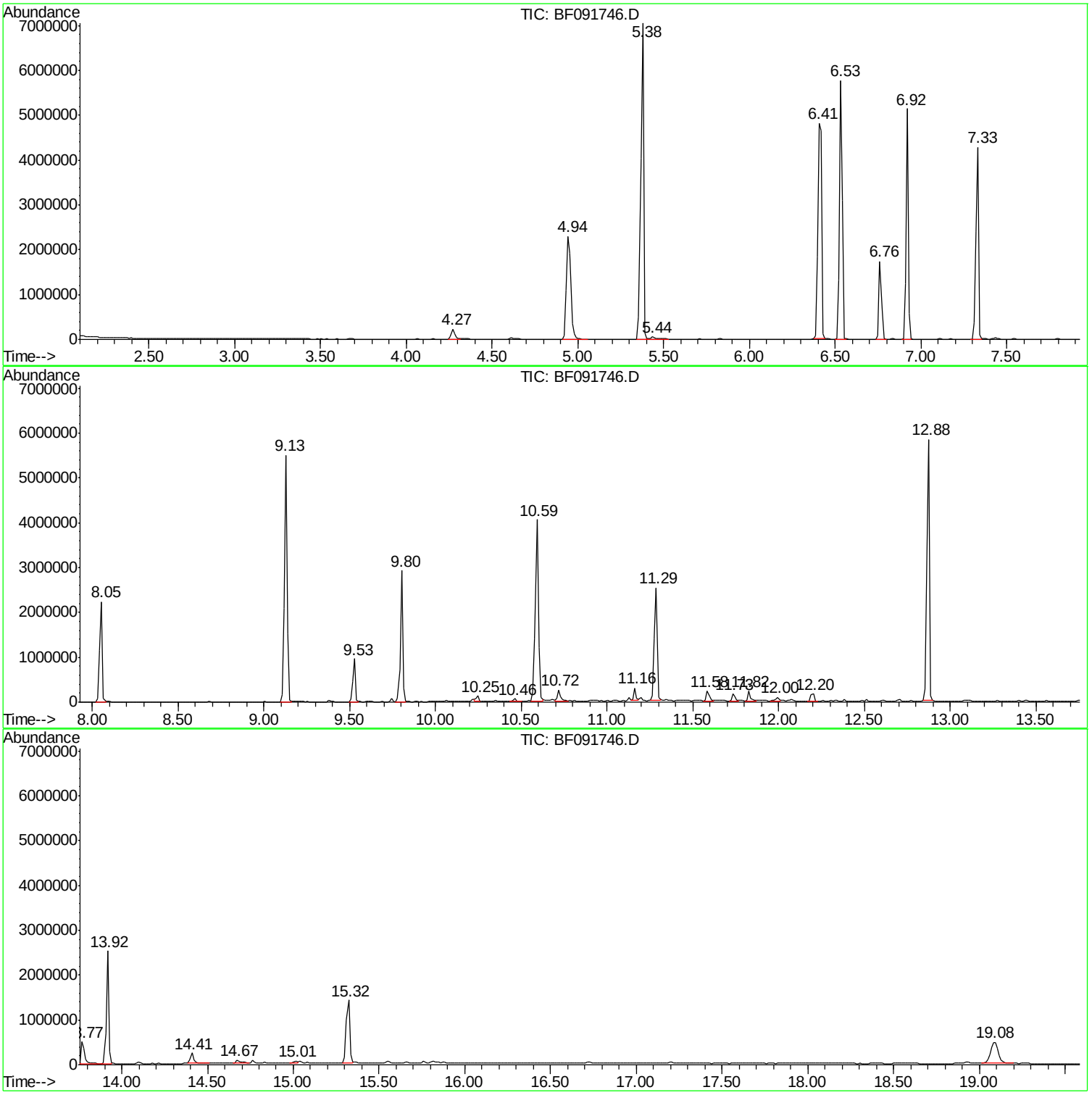
Sum of corrected areas: 74058403

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

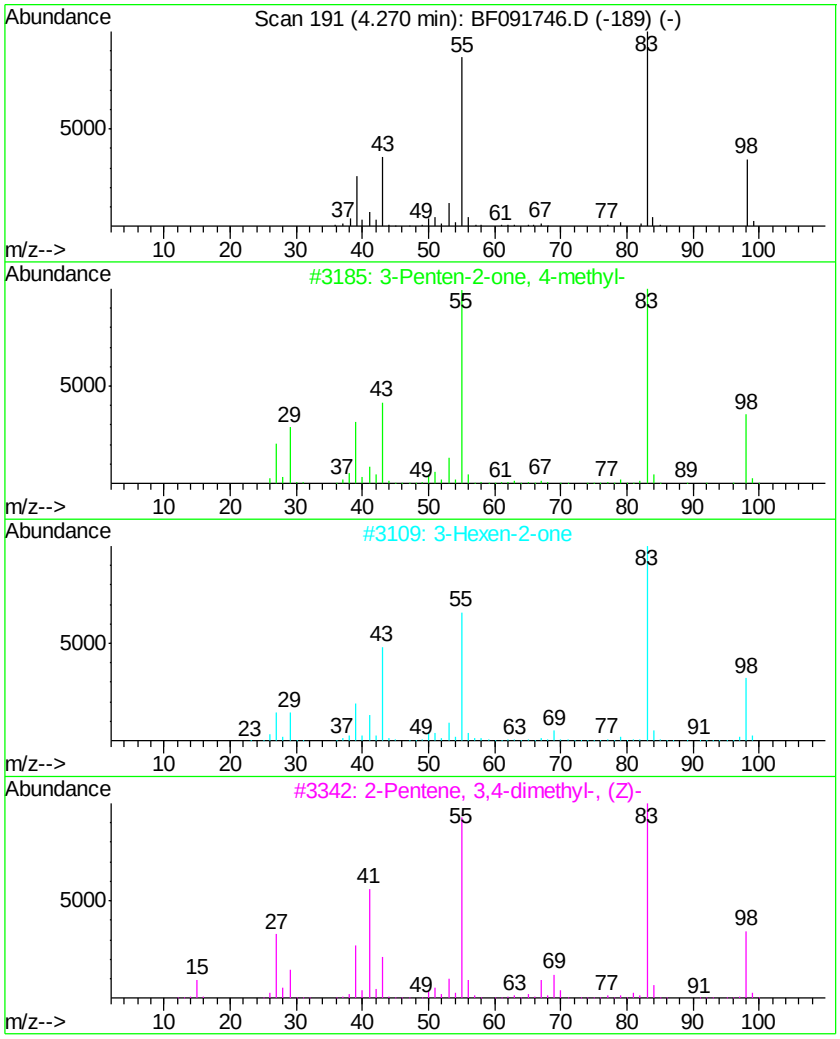
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

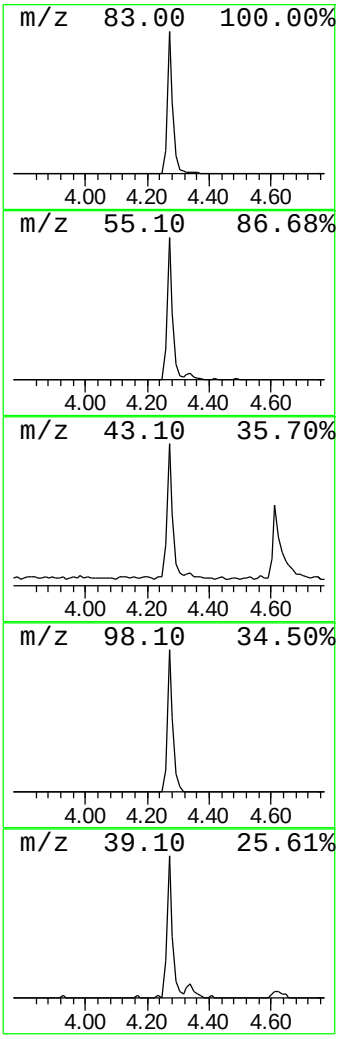
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	3.36 ng	281610	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

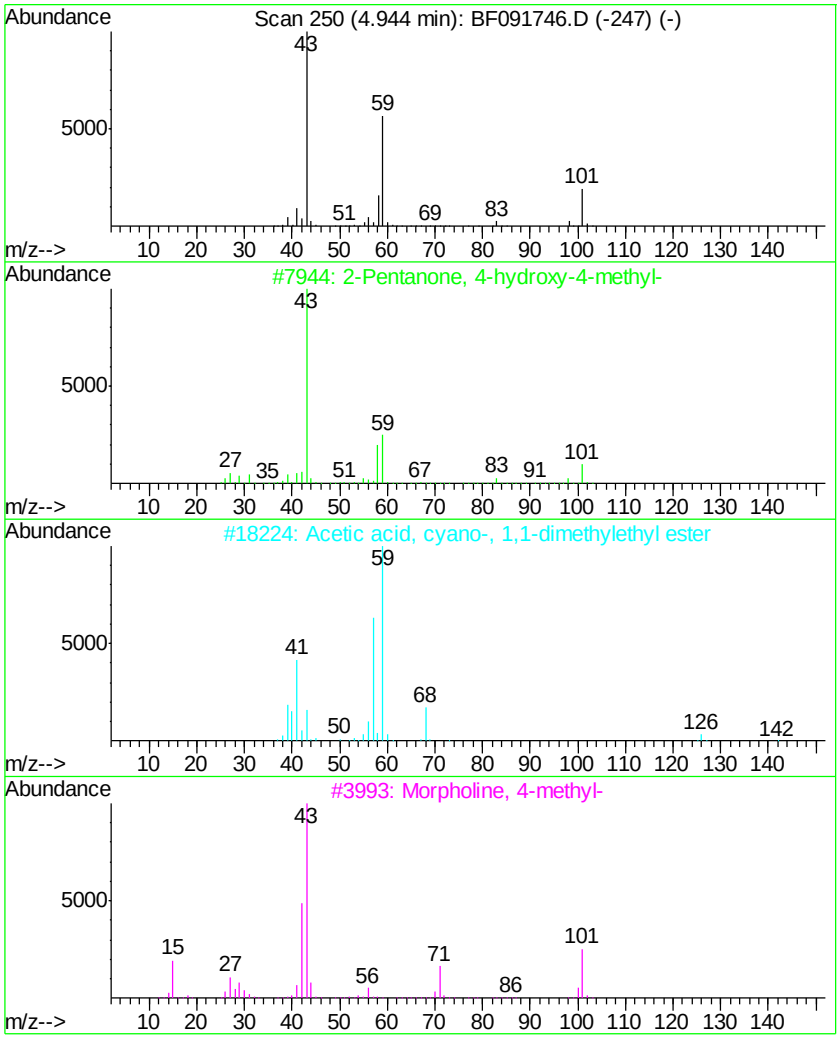
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

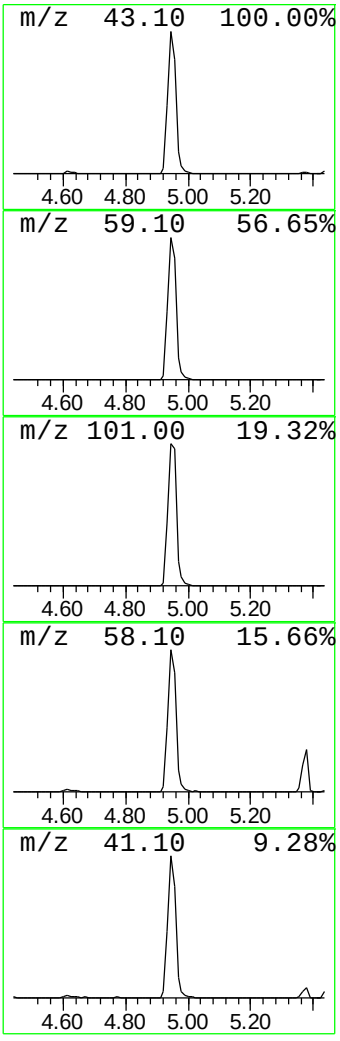
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	48.43 ng	4060270	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

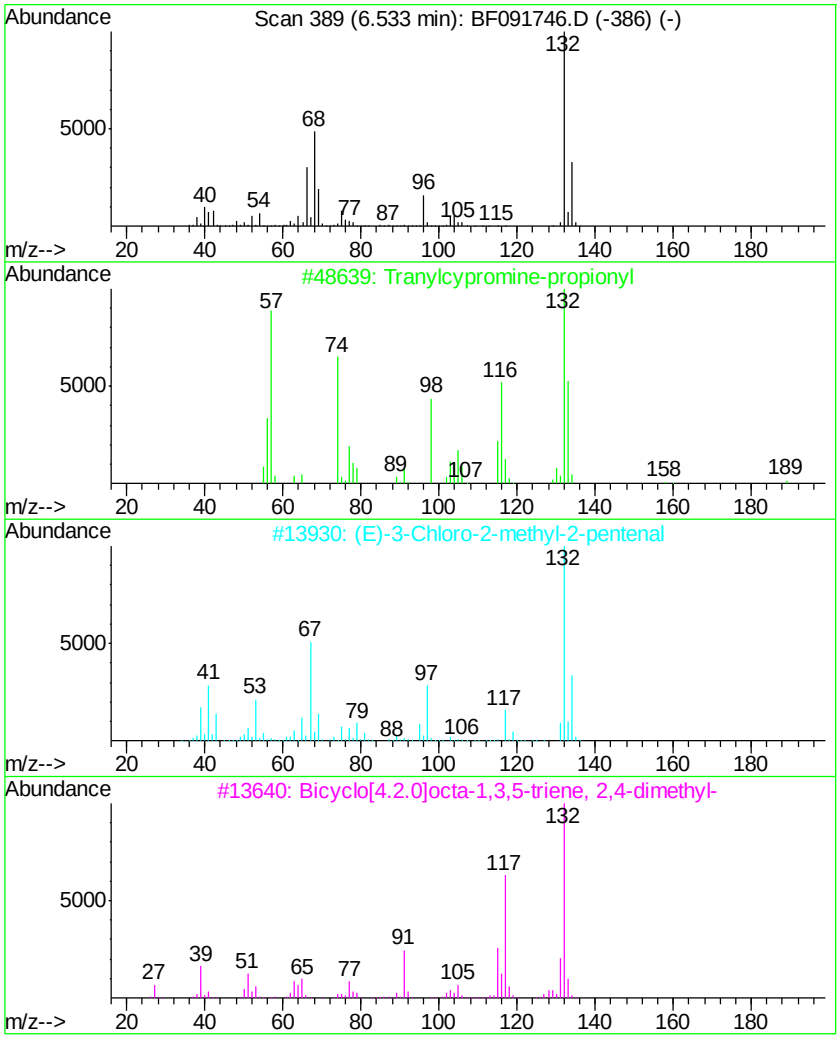
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

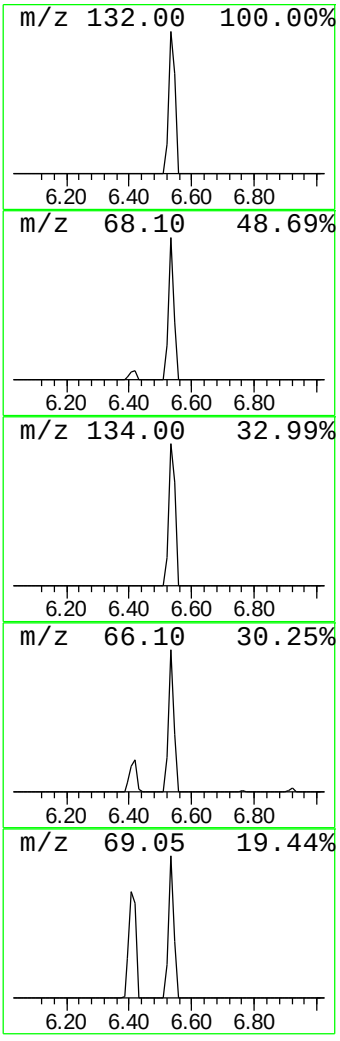
****

Peak Number 3 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	83.54 ng	7004000	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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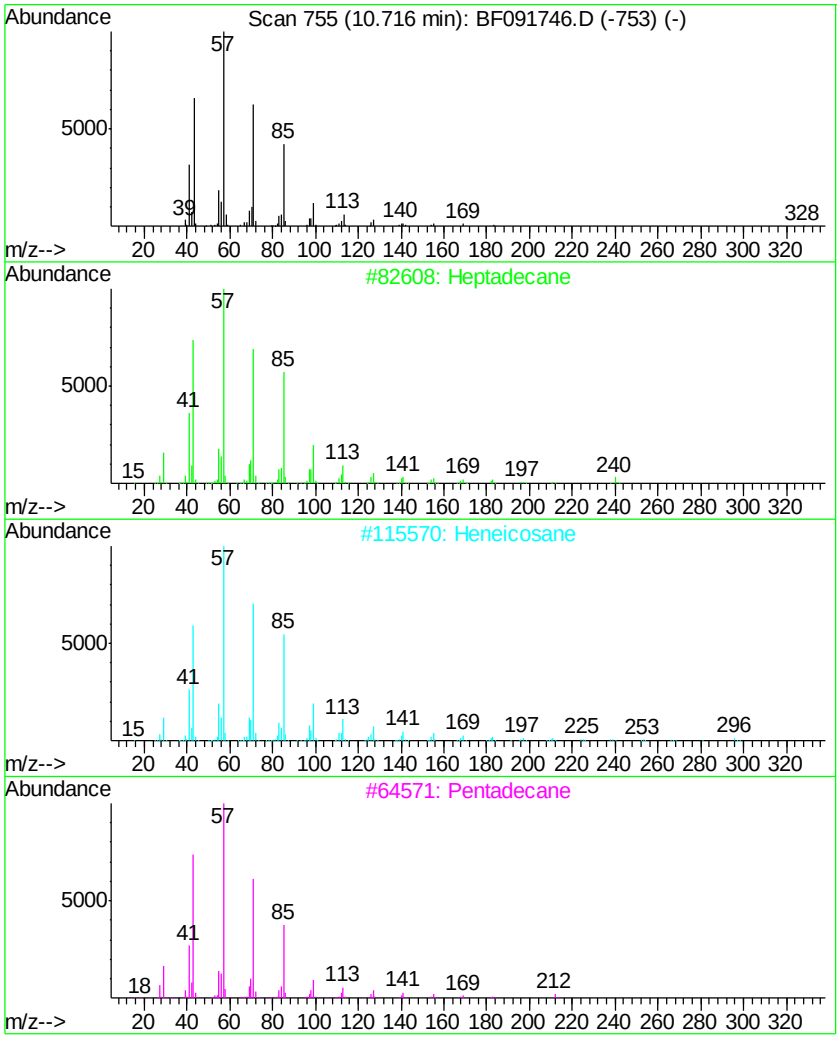
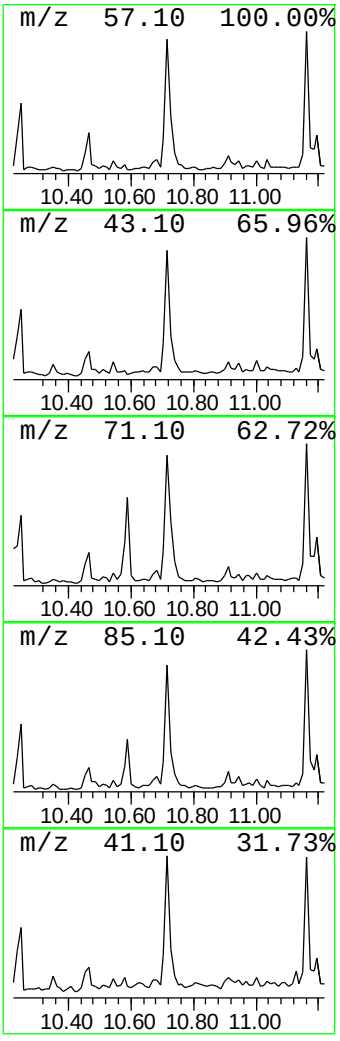
****

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.15 ng	299299	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tridecane	184	C13H28	000629-50-5	83





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Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

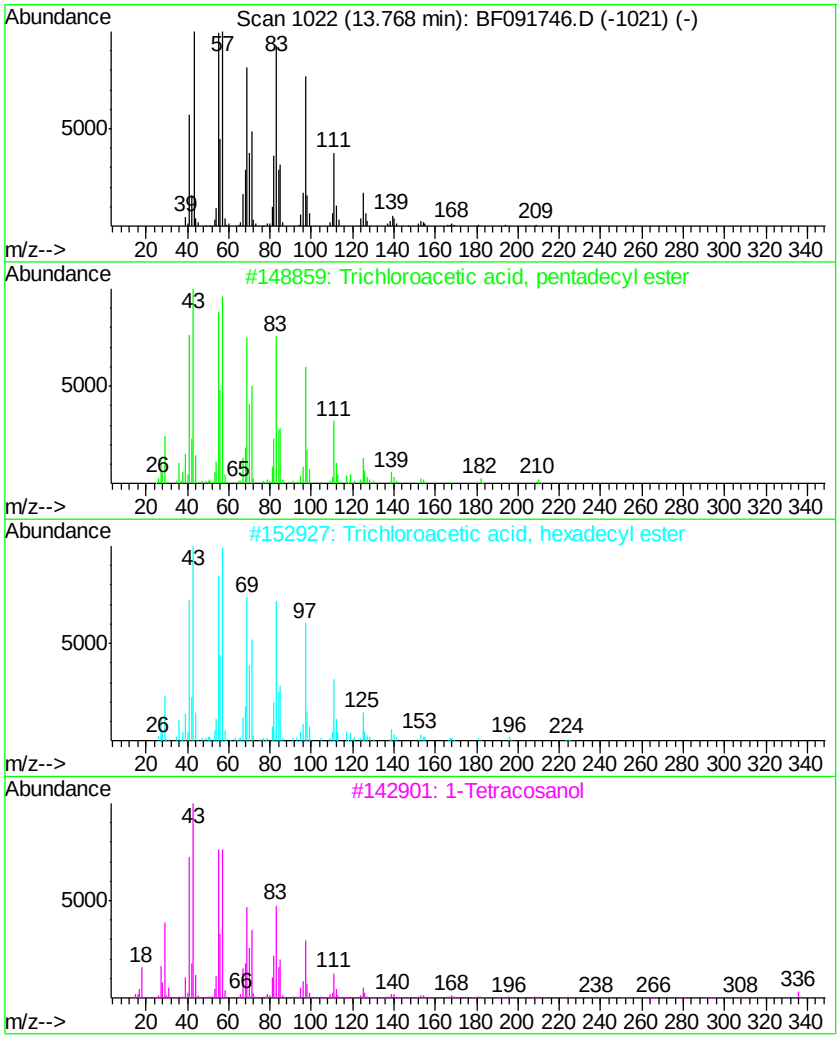
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

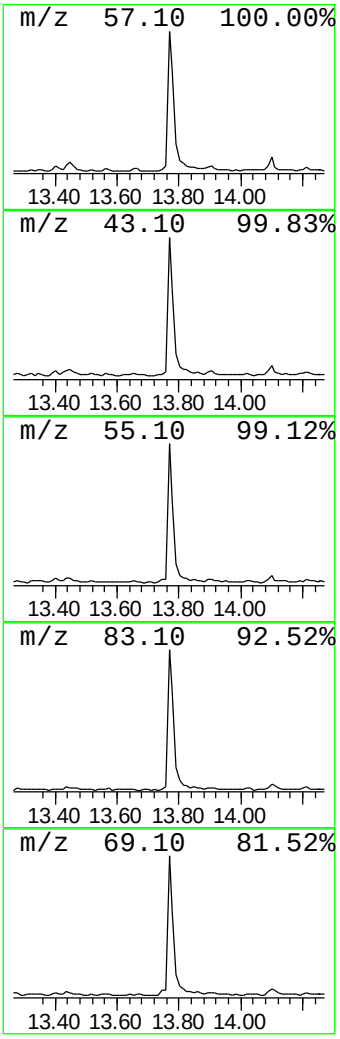
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	5.72 ng	687382	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Tetracosanol	354	C24H50O	000506-51-4	90
4	11-Tricosene	322	C23H46	052078-56-5	86
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





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Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

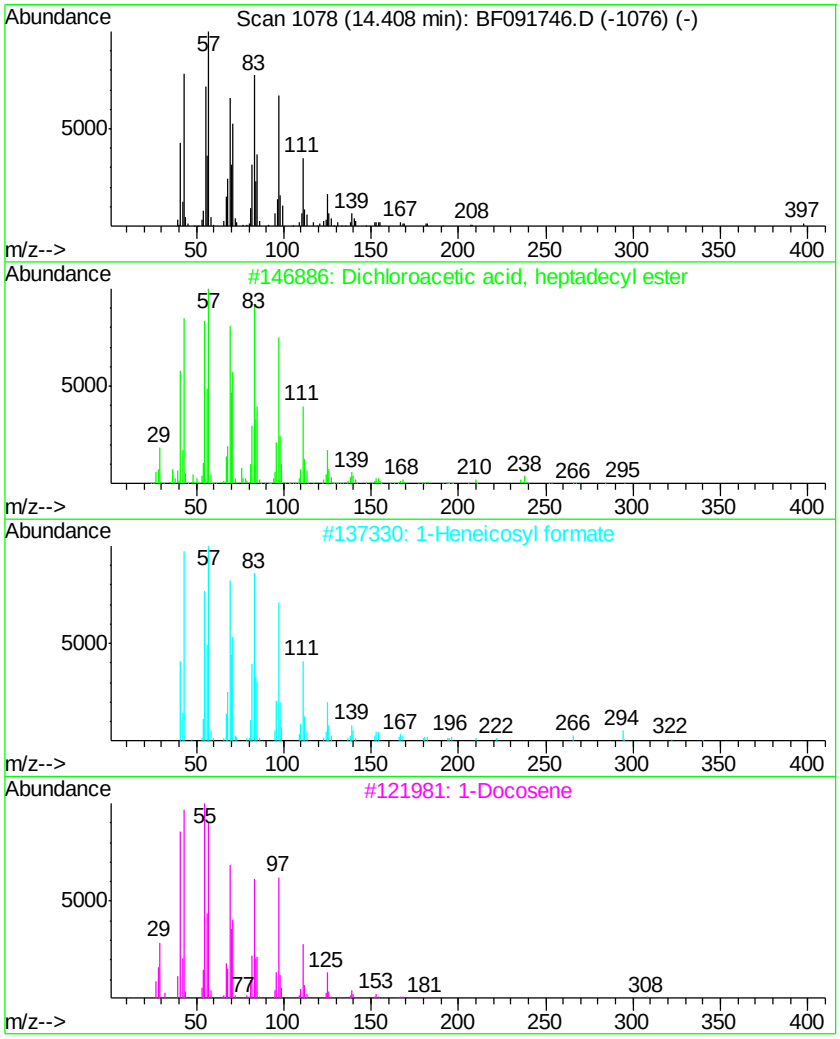
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

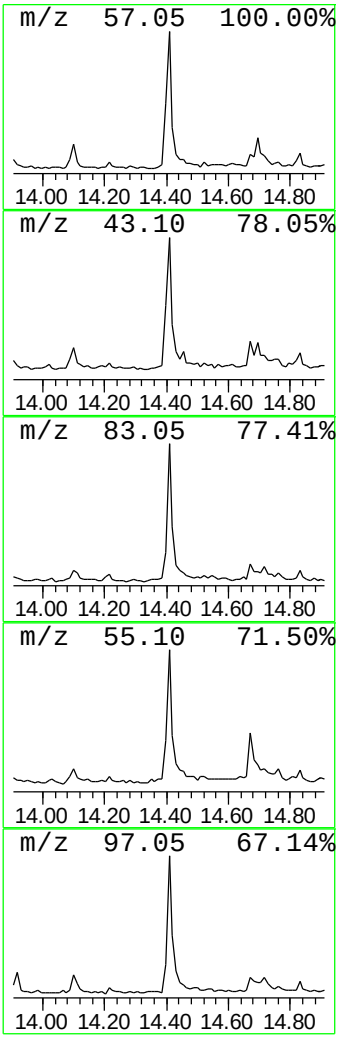
****

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.60 ng	312317	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	1-Docosene	308	C22H44	001599-67-3	91
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	1-Tricosene	322	C23H46	018835-32-0	91





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Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

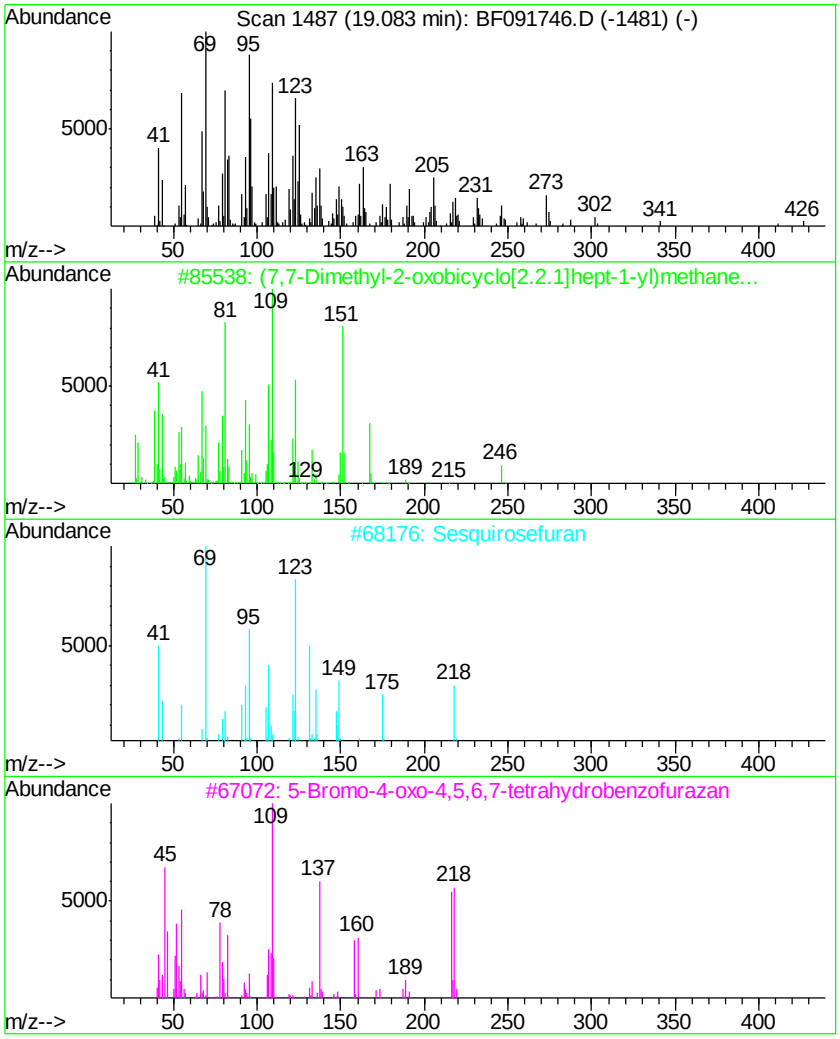
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

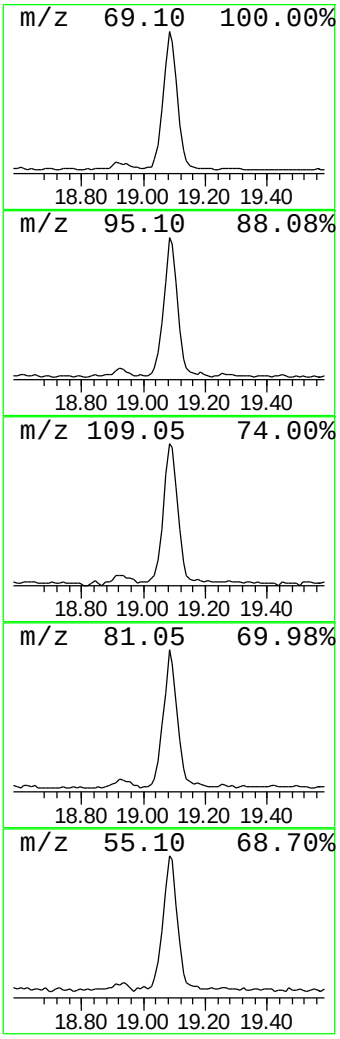
****

Peak Number 8 (7,7-Dimethyl-2-oxobicyclo[... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.08	16.44 ng	1540690	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	246	C11H18O4S	1000197-55-6	70
2	Sesquirosefuran	218	C15H22O	039007-93-7	59
3	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
4	3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	44
5	Bicyclo[3.1.1]heptan-3-one, 2-(b...	192	C13H20O	1000163-96-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121816\
Data File : BF091746.D
Acq On : 18 Dec 2016 19:47
Operator : UM/SJ
Sample : H6099-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP08-3.5-4FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	3.4	ng	281610	1	6.76	1676890	20.0
2-Pentanone, 4-hy...	4.94	48.4	ng	4060270	1	6.76	1676890	20.0
unknown6.53	6.53	83.5	ng	7004000	1	6.76	1676890	20.0
Heptadecane	10.72	2.1	ng	299299	4	11.29	2779550	20.0
Trichloroacetic a...	13.77	5.7	ng	687382	5	13.92	2402910	20.0
Dichloroacetic ac...	14.41	2.6	ng	312317	5	13.92	2402910	20.0
(7,7-Dimethyl-2-o...	19.08	16.4	ng	1540690	6	15.32	1874810	20.0