LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091289.D
Acq On : 23 Nov 2016 21:53
Operator : UM/SJ
Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

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-BF112316.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	1.744	3	5	17	rVB	3225257	5104134	81.18%	8.541%
2	1.904	17	19	40	rVB	3206068	6287252	100.00%	10.520%
3	2.167	40	42	65	rVB4	94788	401997	6.39%	0.673%
4	5.070	293	296	302	rBV	1392289	1940968	30.87%	3.248%
5	5.482	329	332	335	rBV	4006895	4683491	74.49%	7.837%
6	6.510	418	422	424	rBV	4779623	5737978	91.26%	9.601%
7	6.647	431	434	436	rBV	5234957	5025237	79.93%	8.409%
8	6.876	452	454	457	rBV	1488633	1291685	20.54%	2.161%
9	7.036	465	468	470	rBV	4300138	3702677	58.89%	6.196%
10	7.436	500	503	506	rBV	2508783	3008615	47.85%	5.034%
11	8.168	564	567	569	rBV	1582391	1770655	28.16%	2.963%
12	9.242	658	661	664	rBV	5211008	4969659	79.04%	8.316%
13	9.631	693	695	698	rBV	671394	728323	11.58%	1.219%
14	9.916	718	720	722	rVB	2023058	1828300	29.08%	3.059%
15	10.328	755	756	758	rBV	46808	69997	1.11%	0.117%
16	10.705	786	789	791	rBV	3554157	3387747	53.88%	5.669%
17	10.831	798	800	806	rVB	122491	137385	2.19%	0.230%
18	11.276	837	839	841	rBV	141016	130212	2.07%	0.218%
19	11.402	848	850	852	rBV	1970046	1744224	27.74%	2.919%
20	11.631	868	870	872	rBV	194596	163820	2.61%	0.274%
21	11.711	875	877	879	rVB	119194	138847	2.21%	0.232%
22	11.928	894	896	898	rBV	110379	129255	2.06%	0.216%
23	12.111	910	912	915	rVB	94823	84026	1.34%	0.141%
24	12.717	963	965	969	rBV	72439	85178	1.35%	0.143%
25	12.991	986	989	991	rBV	3711132	3914913	62.27%	6.551%
26	13.882	1065	1067	1072	rBV	161392	195667	3.11%	0.327%
27	14.031	1078	1080	1083	rBV	1417728	1258623	20.02%	2.106%
28	14.797	1145	1147	1153	rBV	153547	214108	3.41%	0.358%
29	15.368	1194	1197	1203	rBV3	29386	73545	1.17%	0.123%
30	15.471	1203	1206	1209	rBV	1048422	1254679	19.96%	2.099%
31	15.860	1237	1240	1244	rVB	38817	69987	1.11%	0.117%
32	16.454	1288	1292	1296	rBV	48956	119434	1.90%	0.200%
33	17.163	1351	1354	1361	rVB2	33602	109463	1.74%	0.183%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
SB-02(6-7)

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-BF112316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 59762081

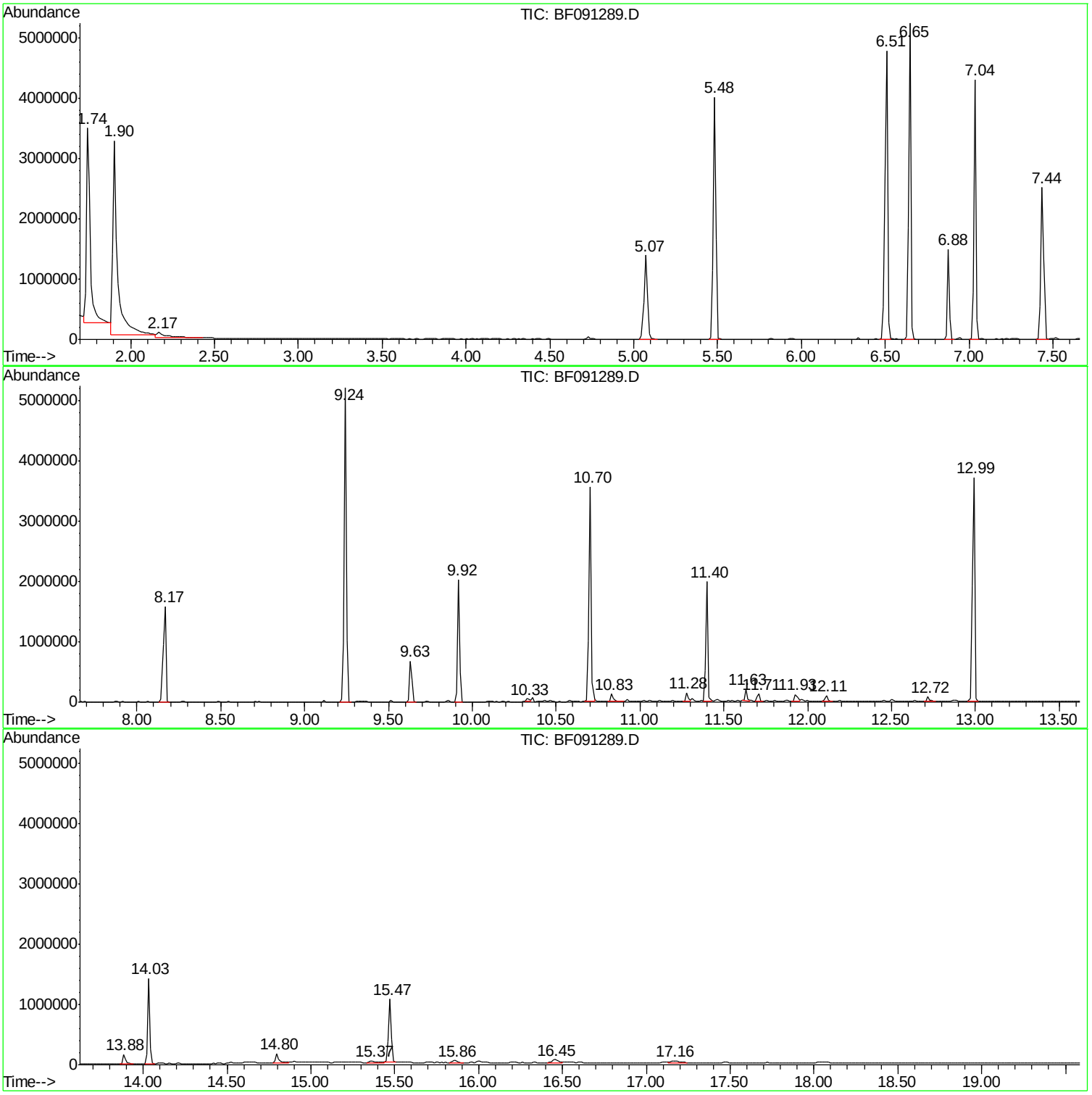
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091289.D
Acq On : 23 Nov 2016 21:53
Operator : UM/SJ
Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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\BF112316\
Data File : BF091289.D
Acq On : 23 Nov 2016 21:53
Operator : UM/SJ
Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

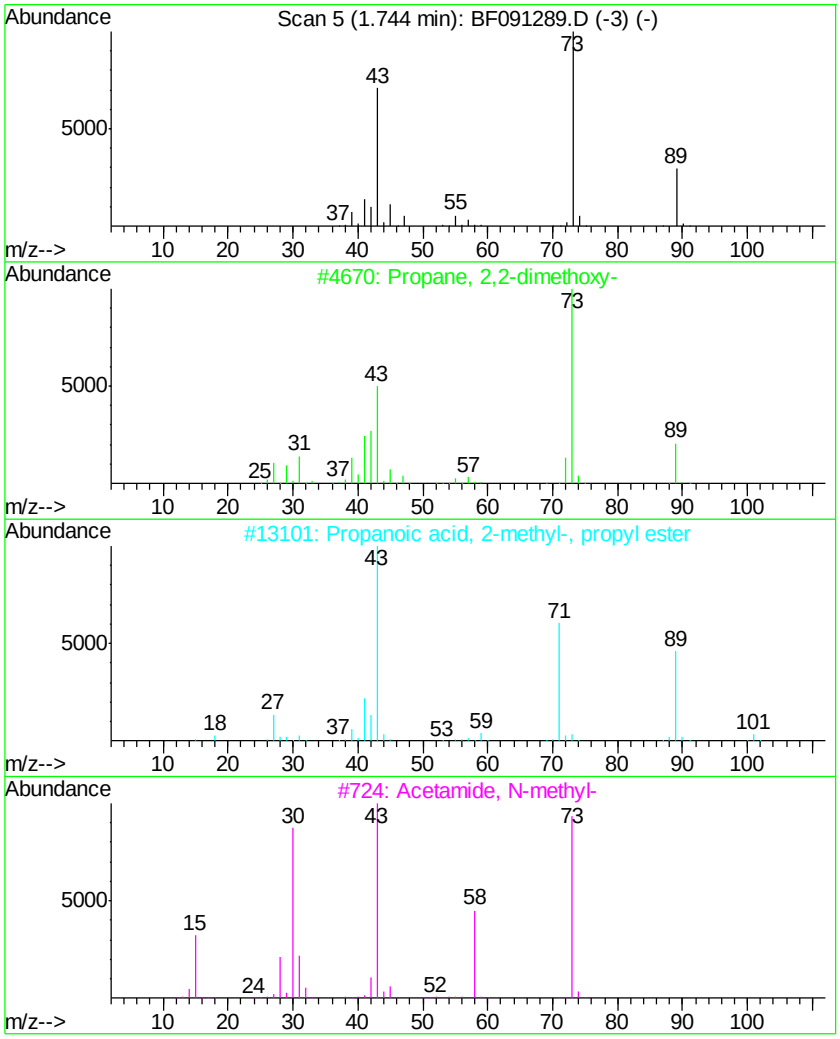
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

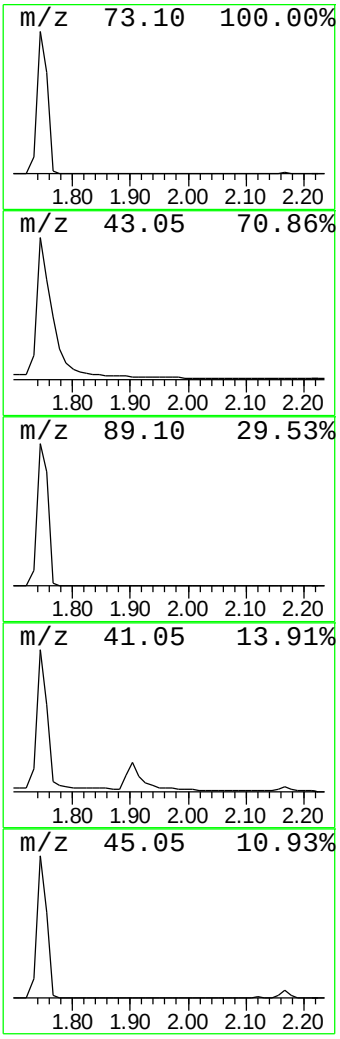
****

Peak Number 1 unknown1.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.74	79.03 ng	5104130	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	17
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091289.D
Acq On : 23 Nov 2016 21:53
Operator : UM/SJ
Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

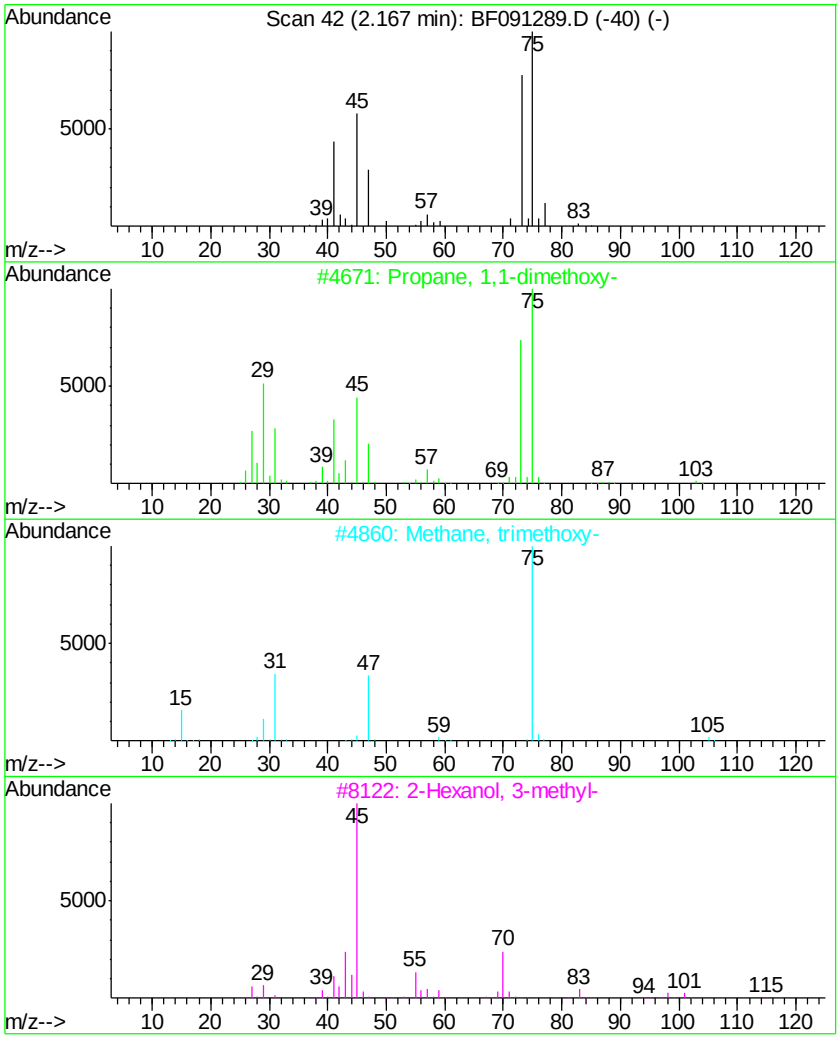
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

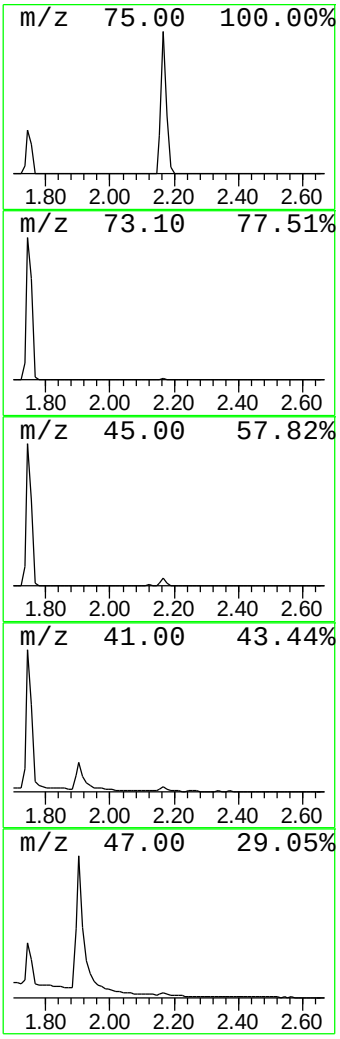
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	6.22 ng	401997	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	Methane, trimethoxy-	106	C4H10O3	000149-73-5	9
3	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	7





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Data File : BF091289.D
Acq On : 23 Nov 2016 21:53
Operator : UM/SJ
Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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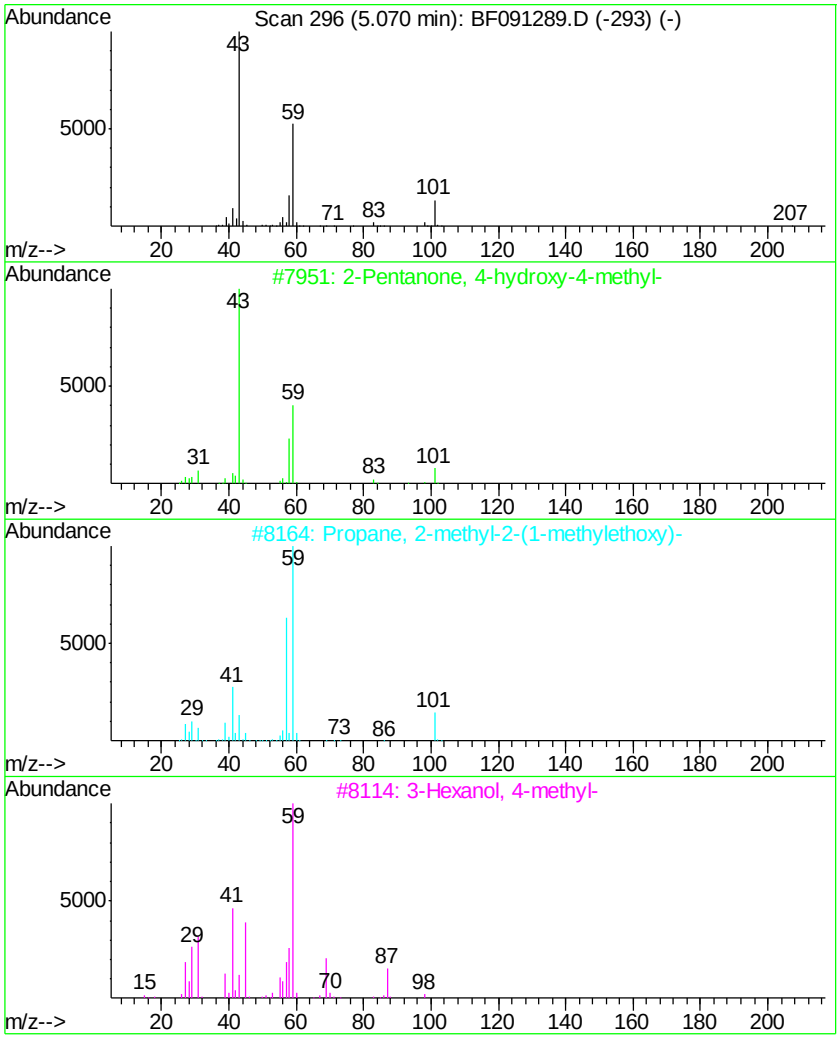
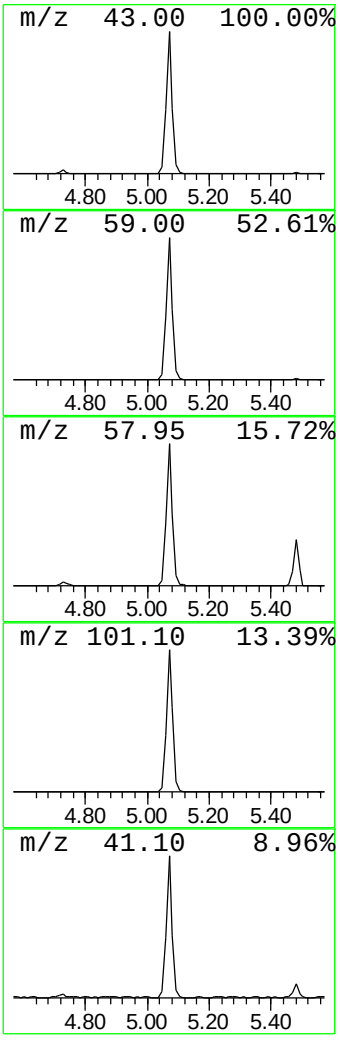
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	30.05 ng	1940970	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Sample : H5740-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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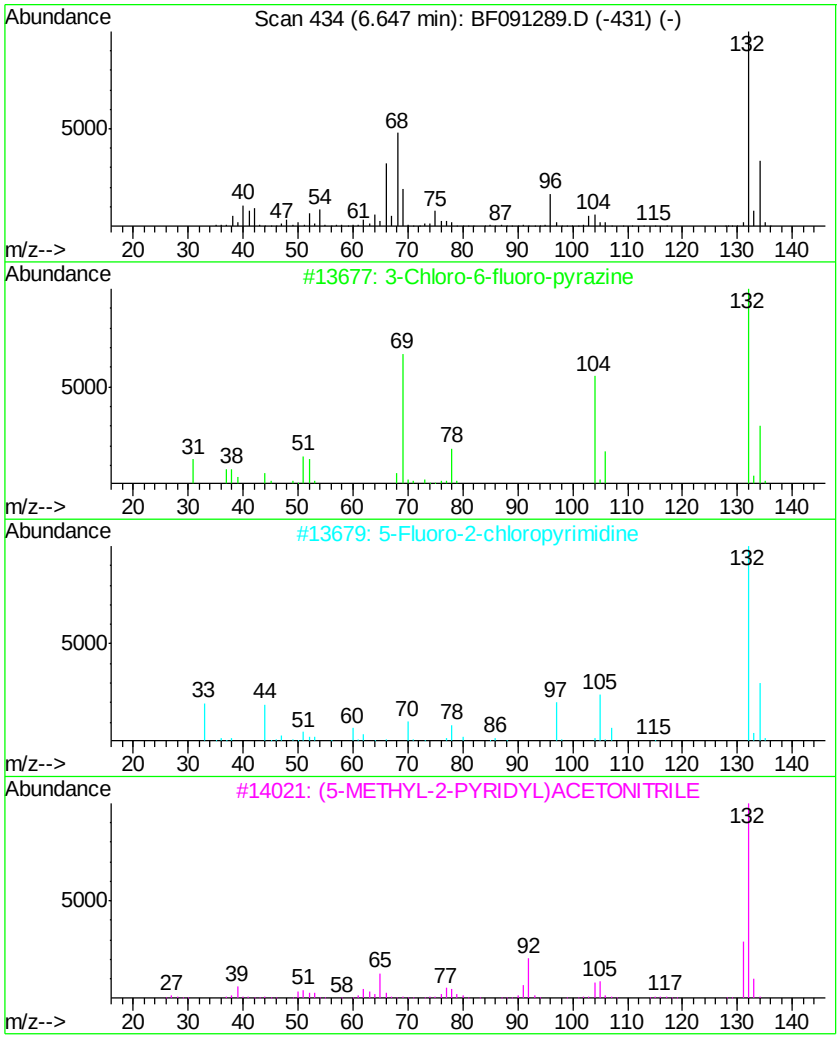
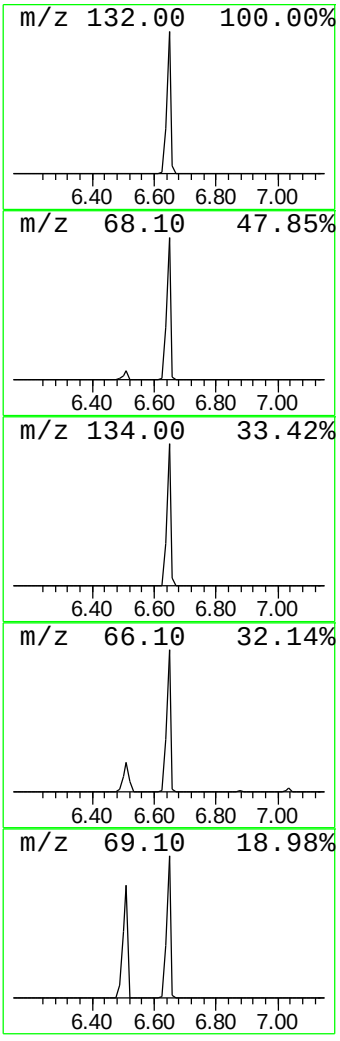
****

Peak Number 5 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	77.81 ng	5025240	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Sample : H5740-05
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Instrument : BNA_F
ClientSampleId : SB-02(6-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

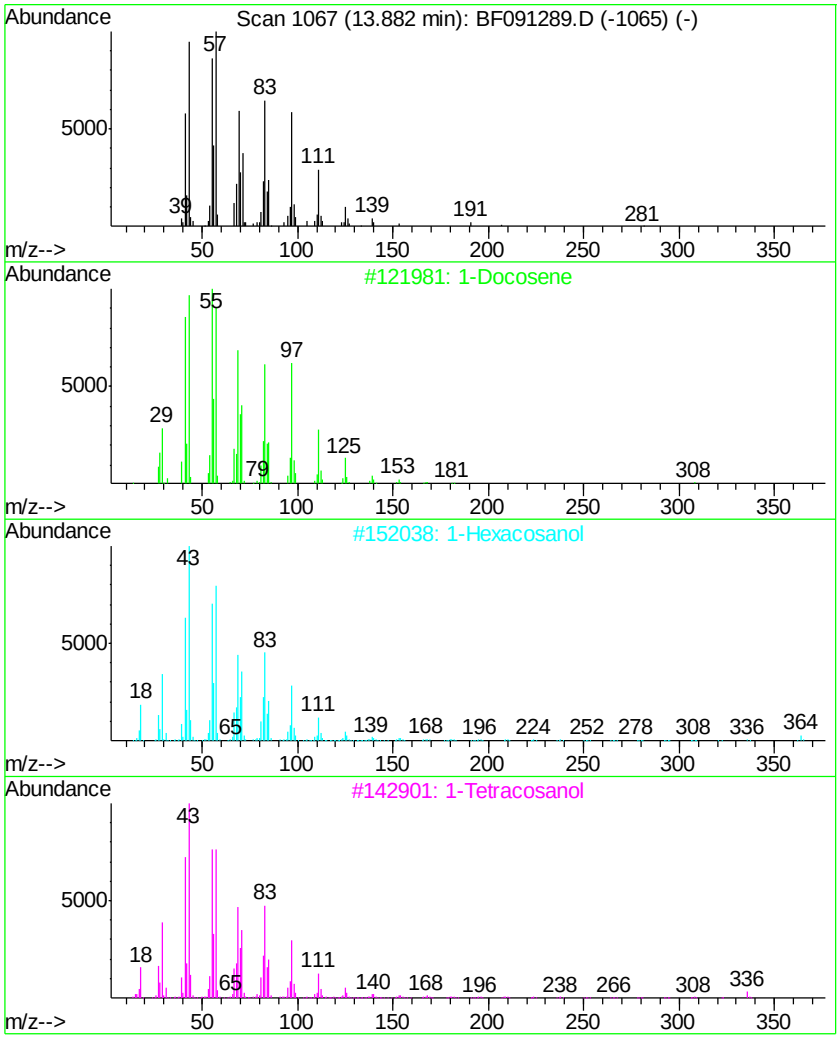
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

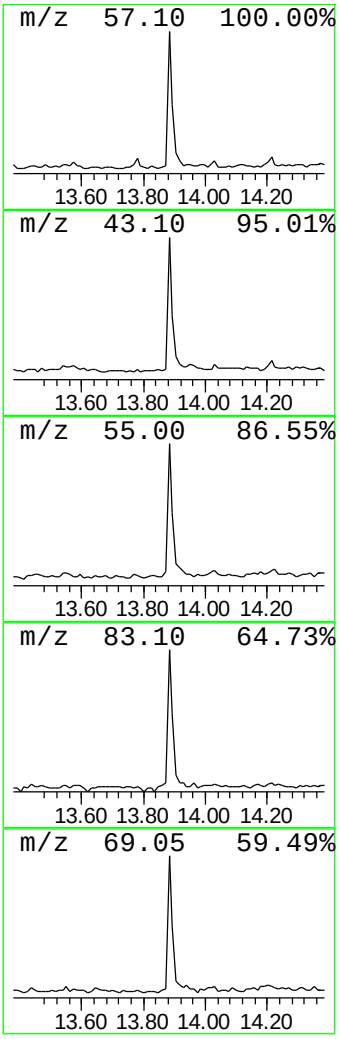
****

Peak Number 7 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.11 ng	195667	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Hexacosanol	382	C26H54O	000506-52-5	87
3	1-Tetracosanol	354	C24H50O	000506-51-4	87
4	17-Pentatriacontene	491	C35H70	006971-40-0	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
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TIC Library : C:\DATABASE\NIST02.L
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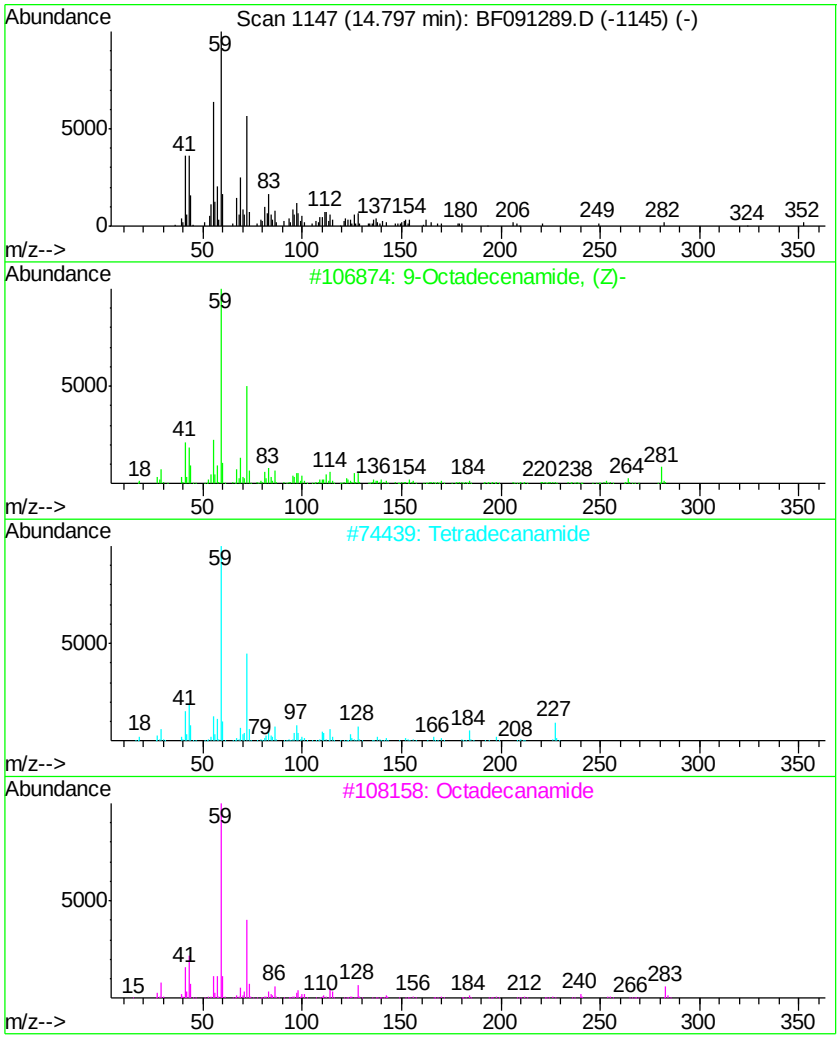
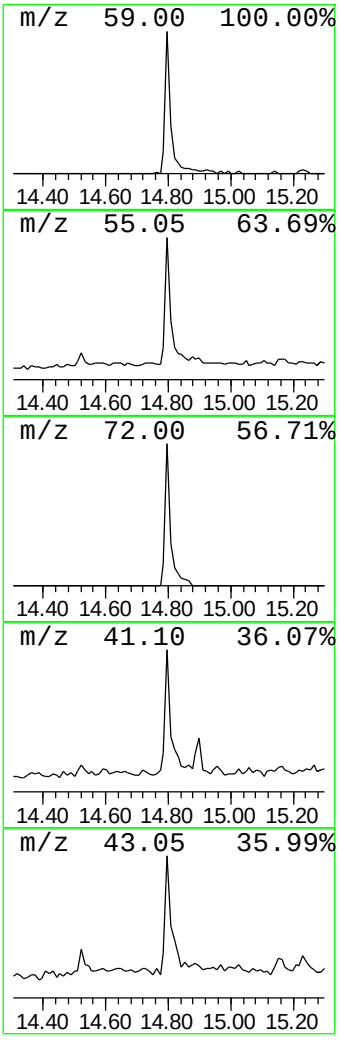
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.41 ng	214108	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Octadecanamide	283	C18H37NO	000124-26-5	80
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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
unknown1.74	1.74	79.0	ng	5104130	1	6.88	1291690	20.0
Propane, 1,1-dime...	2.17	6.2	ng	401997	1	6.88	1291690	20.0
2-Pentanone, 4-hy...	5.07	30.1	ng	1940970	1	6.88	1291690	20.0
unknown6.65	6.65	77.8	ng	5025240	1	6.88	1291690	20.0
1-Docosene	13.88	3.1	ng	195667	5	14.03	1258620	20.0
9-Octadecenamide,...	14.80	3.4	ng	214108	6	15.47	1254680	20.0