LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091288.D
Acq On : 23 Nov 2016 21:25
Operator : UM/SJ
Sample : H5740-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01(4-6)

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	1.767	4	7	9	rBV	4528987	6197477	97.68%	9.403%
2	1.904	17	19	41	rVB	2585369	5391567	84.98%	8.180%
3	2.178	41	43	55	rVB2	86913	201797	3.18%	0.306%
4	5.070	293	296	302	rBV	1251826	2157071	34.00%	3.273%
5	5.493	329	333	335	rBV	3971368	6087328	95.94%	9.235%
6	6.510	418	422	425	rVB	5043819	6344672	100.00%	9.626%
7	6.647	431	434	436	rBV	5495027	5364435	84.55%	8.139%
8	6.876	452	454	456	rBV	1456363	1294300	20.40%	1.964%
9	7.036	465	468	470	rBV	4592117	4079522	64.30%	6.189%
10	7.436	500	503	506	rBV	2558312	3823292	60.26%	5.801%
11	8.168	564	567	569	rBV	1580648	1780447	28.06%	2.701%
12	9.196	655	657	658	rBV	498457	392561	6.19%	0.596%
13	9.242	658	661	664	rVB	5430919	5395073	85.03%	8.185%
14	9.631	693	695	698	rBV	592318	622244	9.81%	0.944%
15	9.916	718	720	722	rVB	2047776	1844909	29.08%	2.799%
16	10.705	786	789	791	rBV	3898114	3794051	59.80%	5.756%
17	10.831	799	800	804	rVB	134994	146151	2.30%	0.222%
18	11.276	837	839	841	rBV	160594	143674	2.26%	0.218%
19	11.402	848	850	852	rBV	2021751	1742208	27.46%	2.643%
20	11.711	874	877	879	rBV	112850	137440	2.17%	0.209%
21	11.939	894	897	899	rBV	398896	508652	8.02%	0.772%
22	12.637	953	958	963	rBV5	43650	143679	2.26%	0.218%
23	12.717	963	965	972	rVV	265076	368878	5.81%	0.560%
24	12.991	986	989	991	rBV	4506728	4452291	70.17%	6.755%
25	13.882	1065	1067	1071	rBV	234695	267606	4.22%	0.406%
26	14.031	1078	1080	1083	rBV	1484541	1307514	20.61%	1.984%
27	14.157	1083	1091	1094	rBV4	65258	294572	4.64%	0.447%
28	14.797	1145	1147	1152	rVB	229302	265643	4.19%	0.403%
29	15.471	1203	1206	1209	rBV	1008583	1247322	19.66%	1.892%
30	19.494	1554	1558	1562	rBV2	28691	116556	1.84%	0.177%

Sum of corrected areas: 65912932

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Data File : BF091288.D
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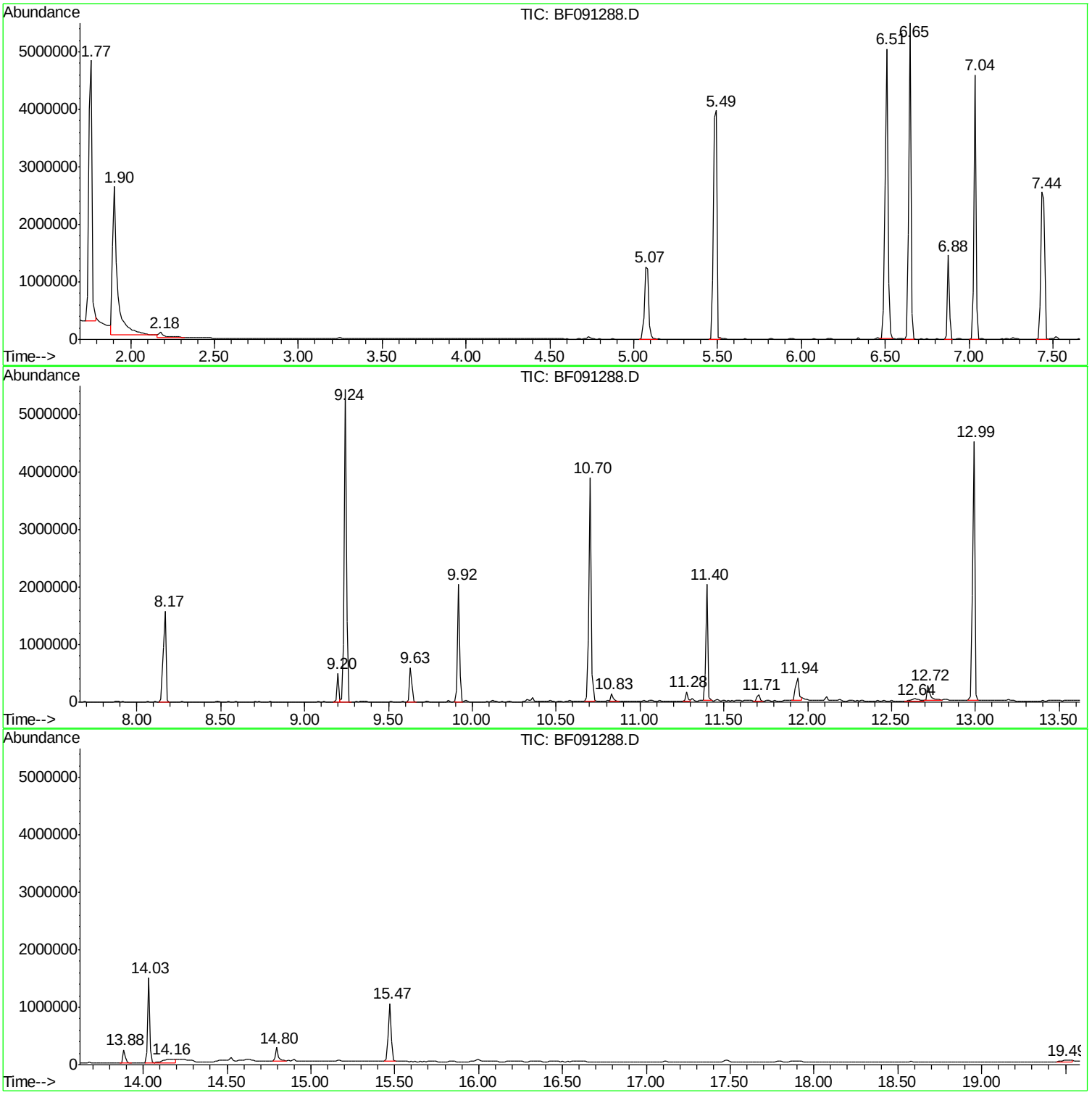
Sample : H5740-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01(4-6)

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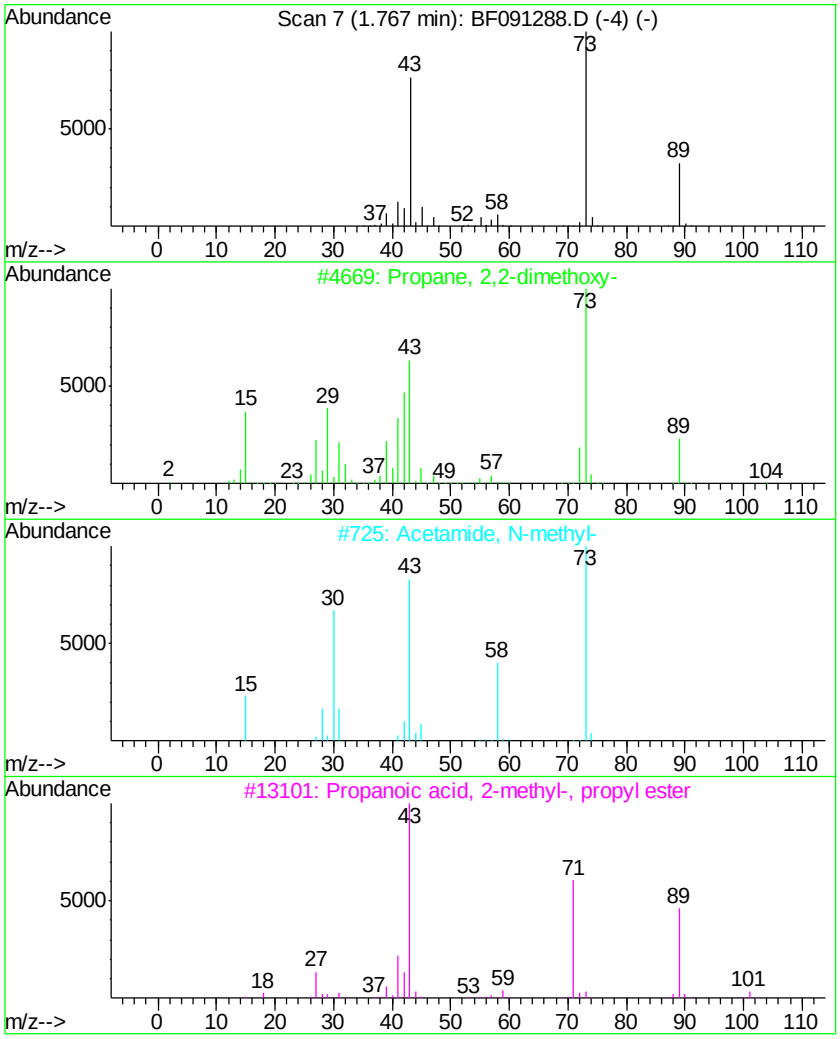
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

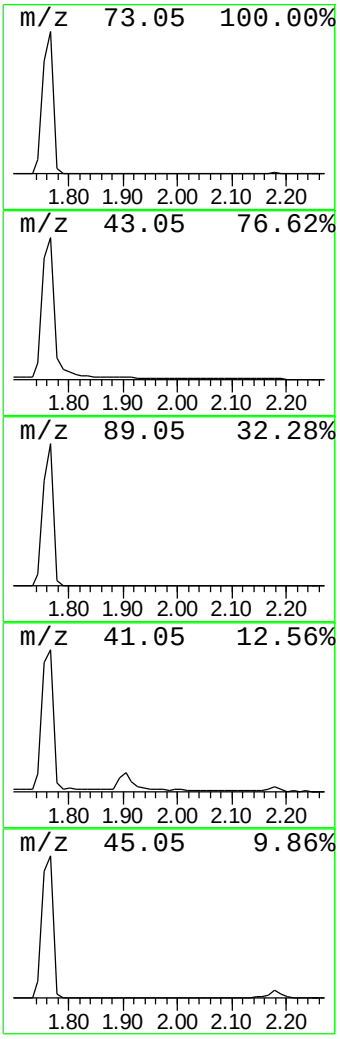
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	95.77 ng	6197480	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	50
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	50
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	25
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SB-01(4-6)

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

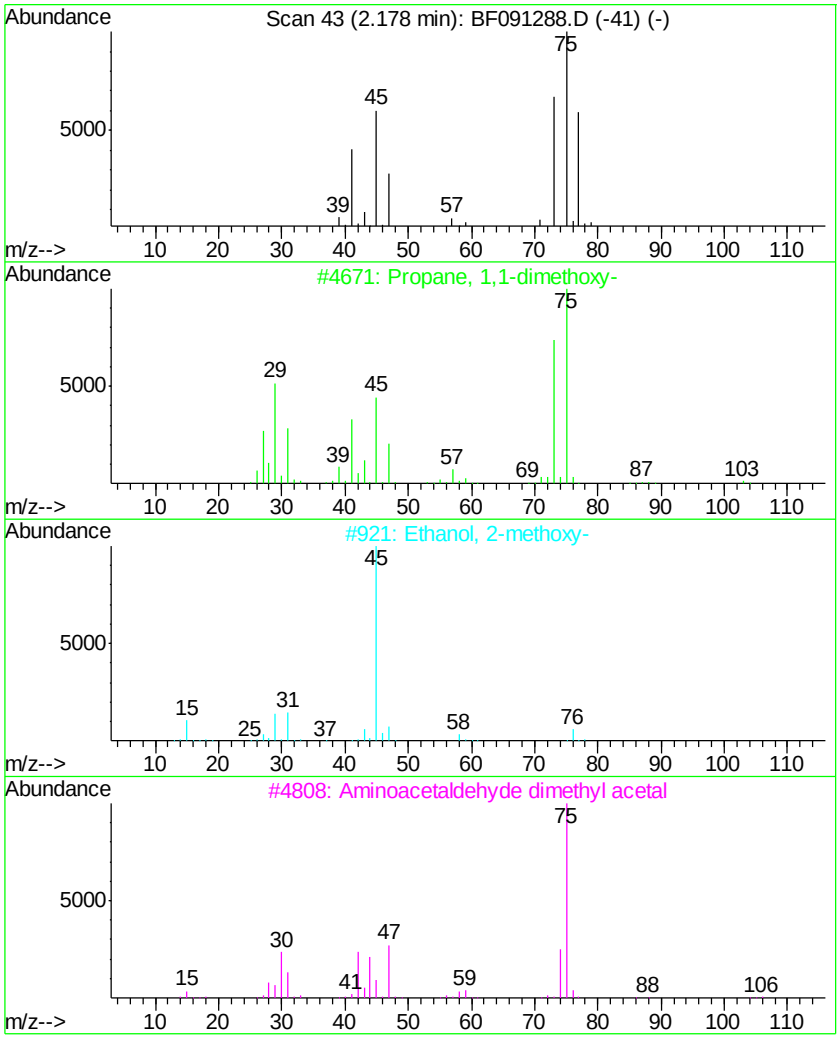
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

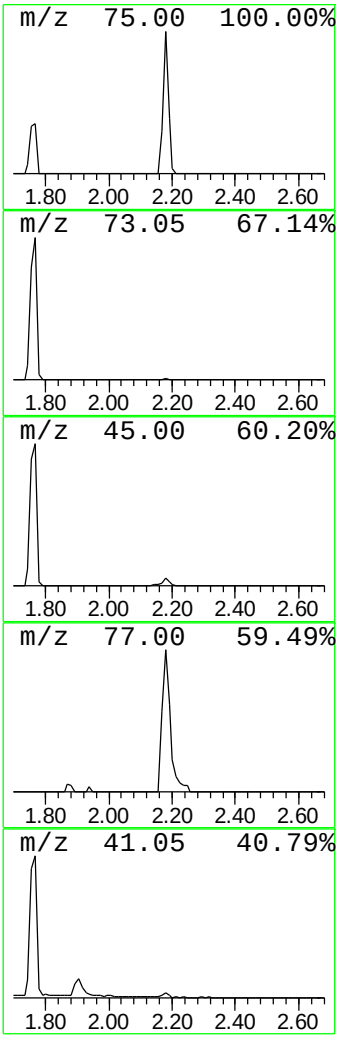
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	3.12 ng	201797	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	59
2	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-01(4-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
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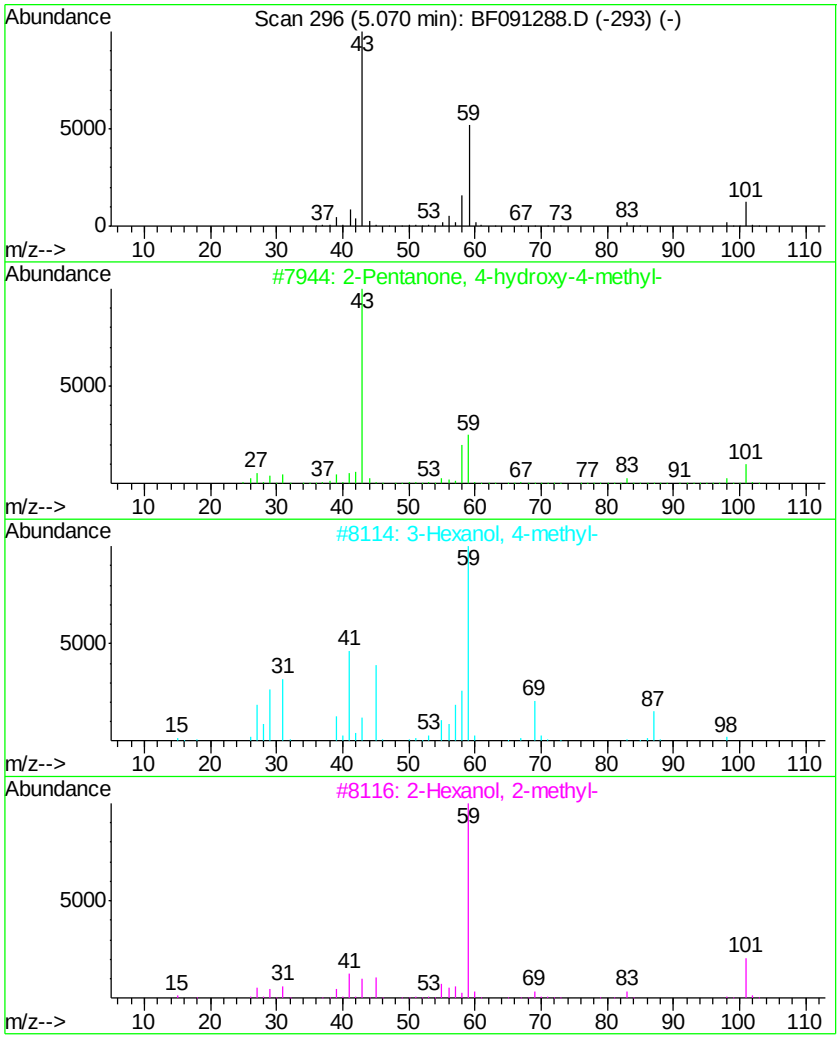
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

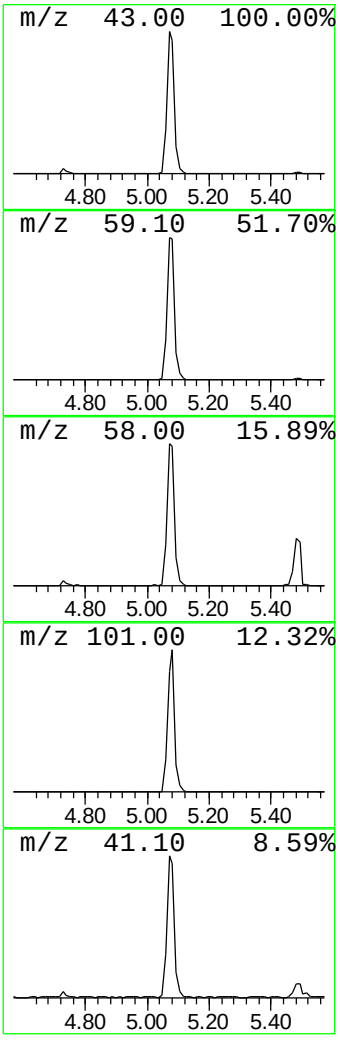
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	33.33 ng	2157070	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	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-01(4-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
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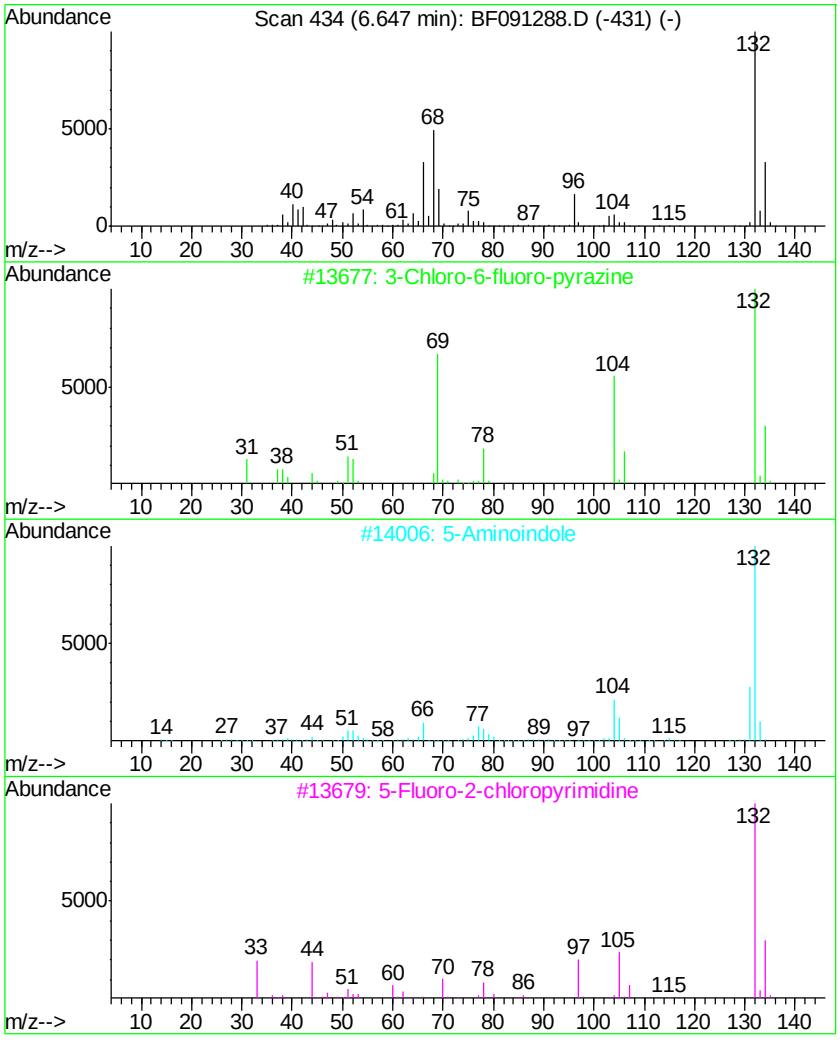
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

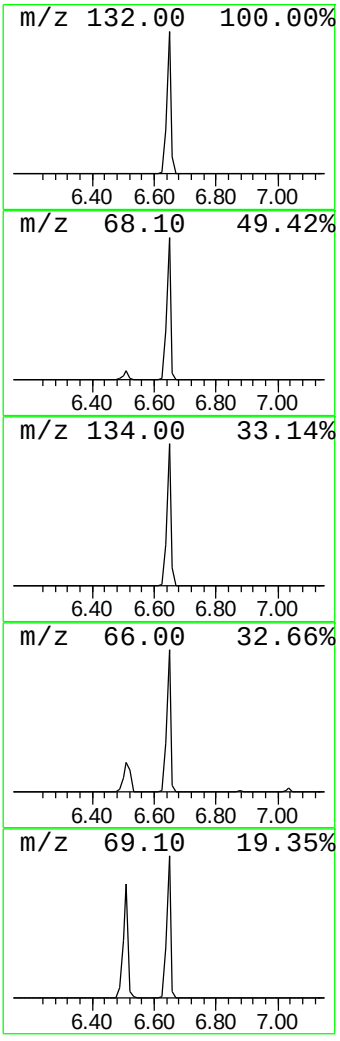
****

Peak Number 5 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	82.89 ng	5364440	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-Aminoindole	132	C8H8N2	005192-03-0	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Sample : H5740-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01(4-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
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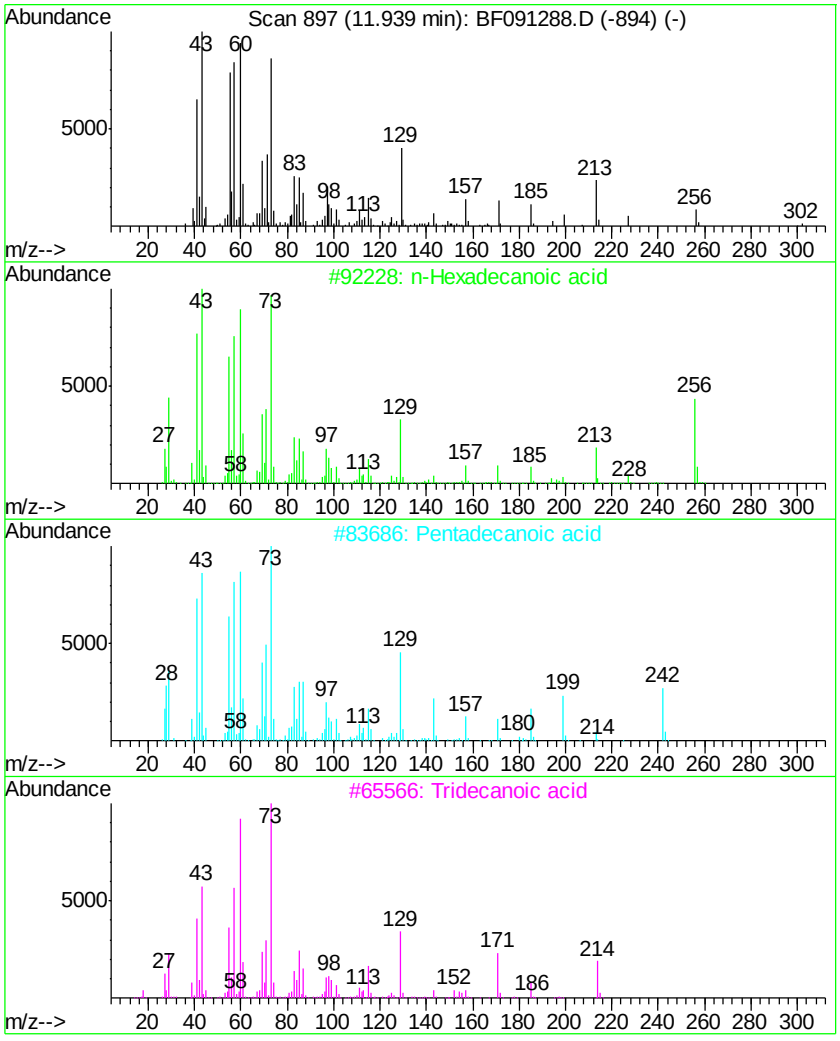
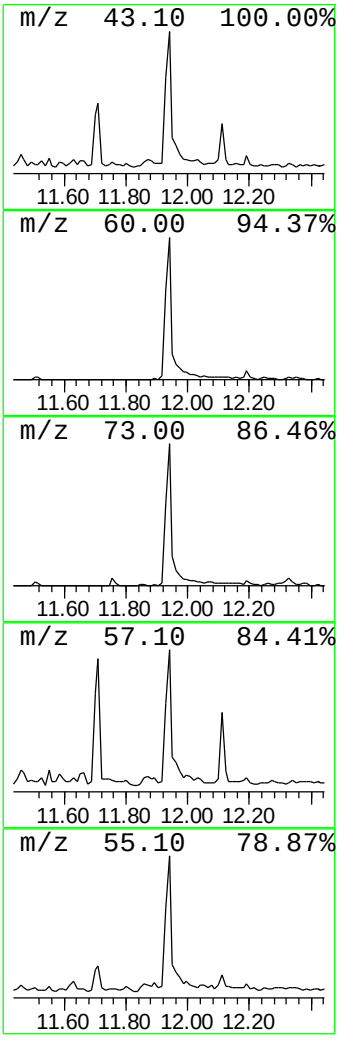
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.84 ng	508652	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01(4-6)

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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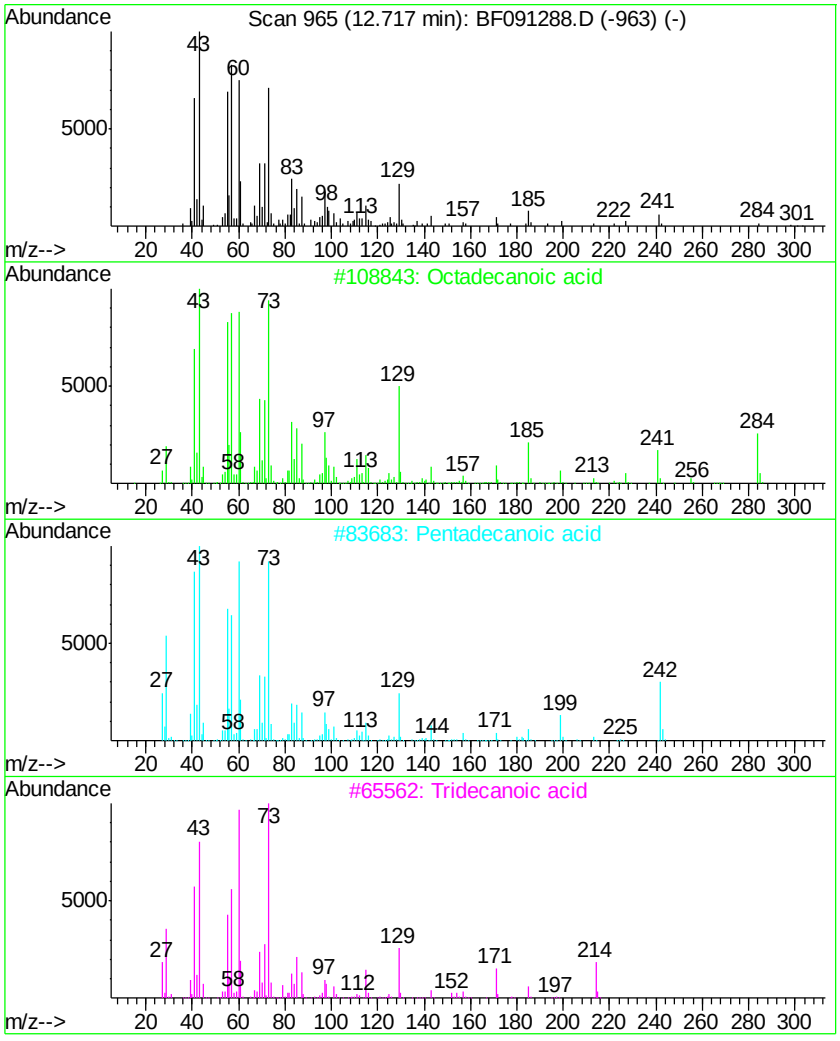
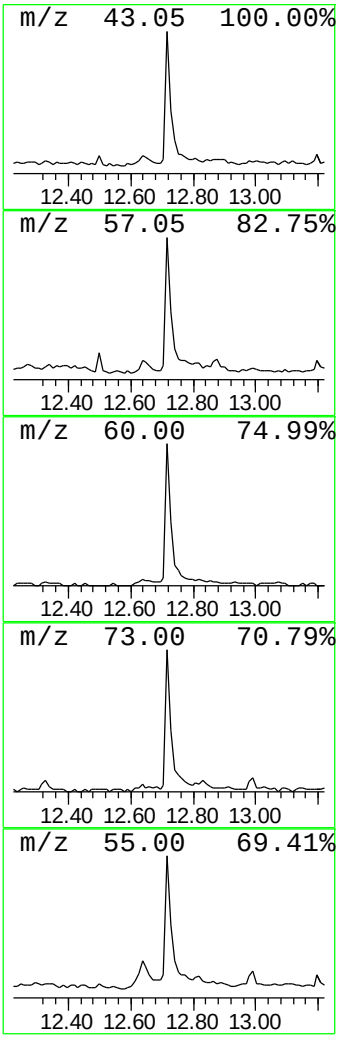
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	4.23 ng	368878	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

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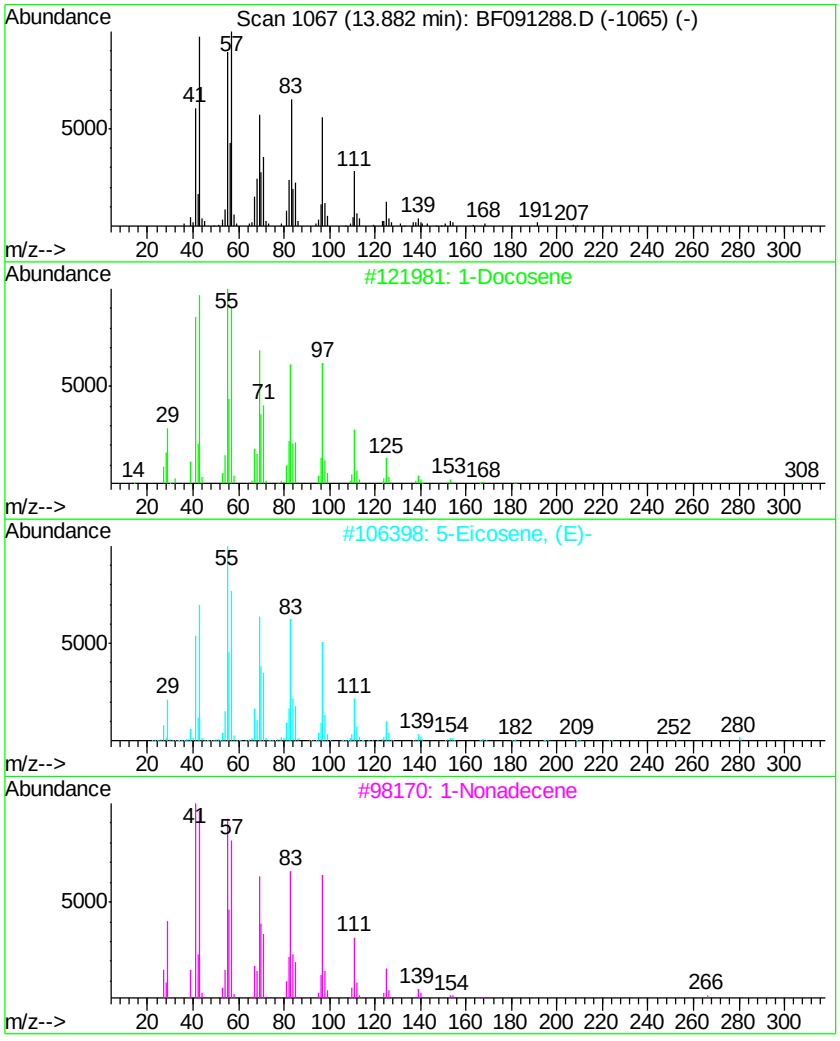
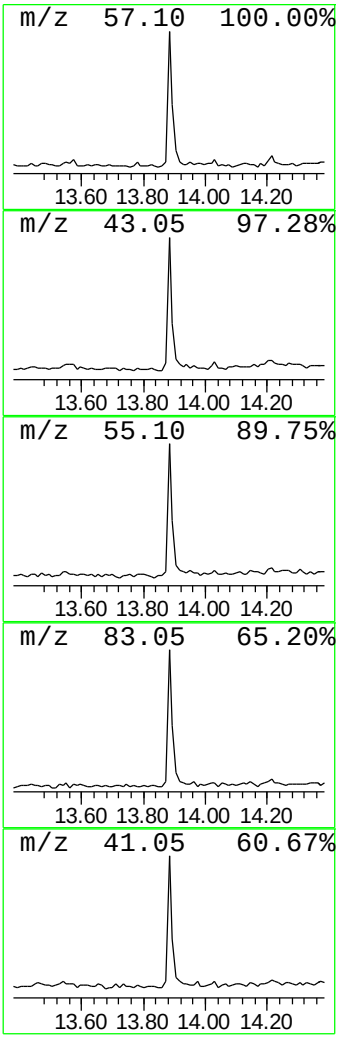
****

Peak Number 9 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	4.09 ng	267606	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	83





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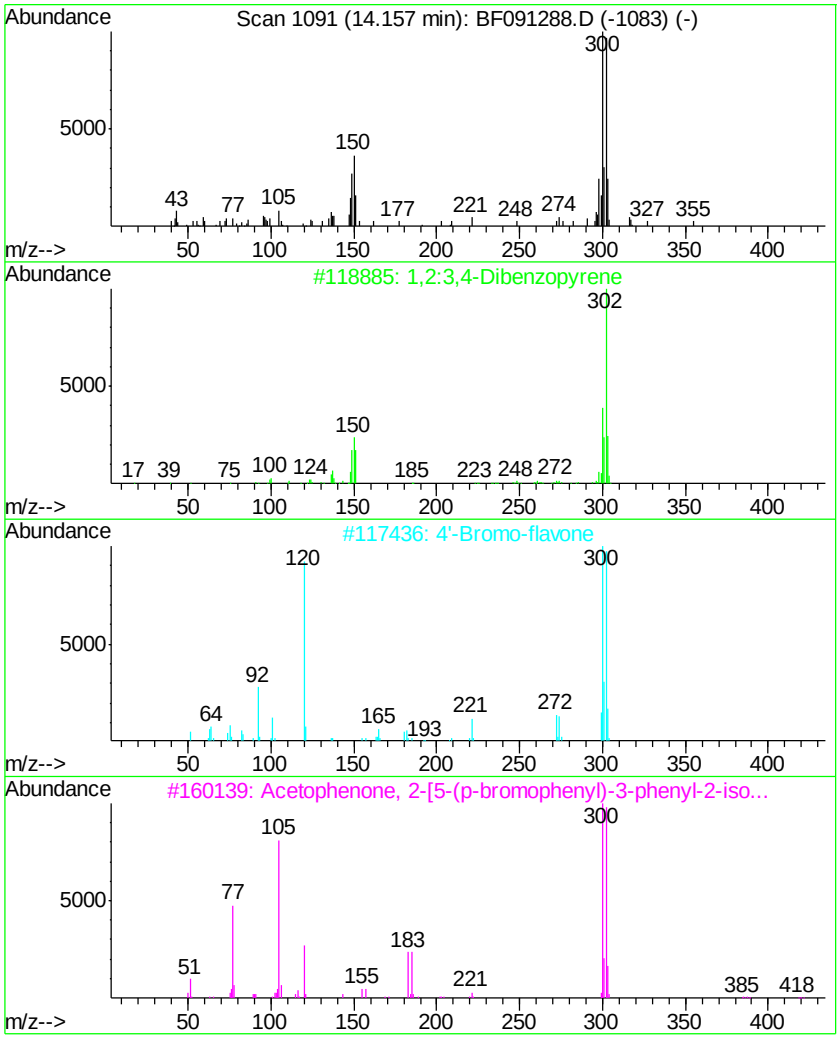
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

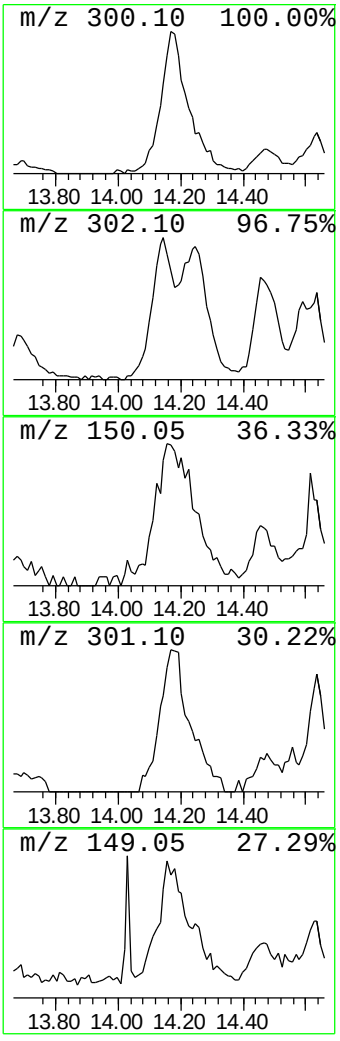
****

Peak Number 10 1,2:3,4-Dibenzopyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	4.51 ng	294572	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	60
2	4'-Bromo-flavone	300	C15H9BrO2	020525-20-6	59
3	Acetophenone, 2-[5-(p-bromopheny...	419	C23H18BrNO2	029809-07-2	59
4	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	55
5	Coronene	300	C24H12	000191-07-1	50





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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

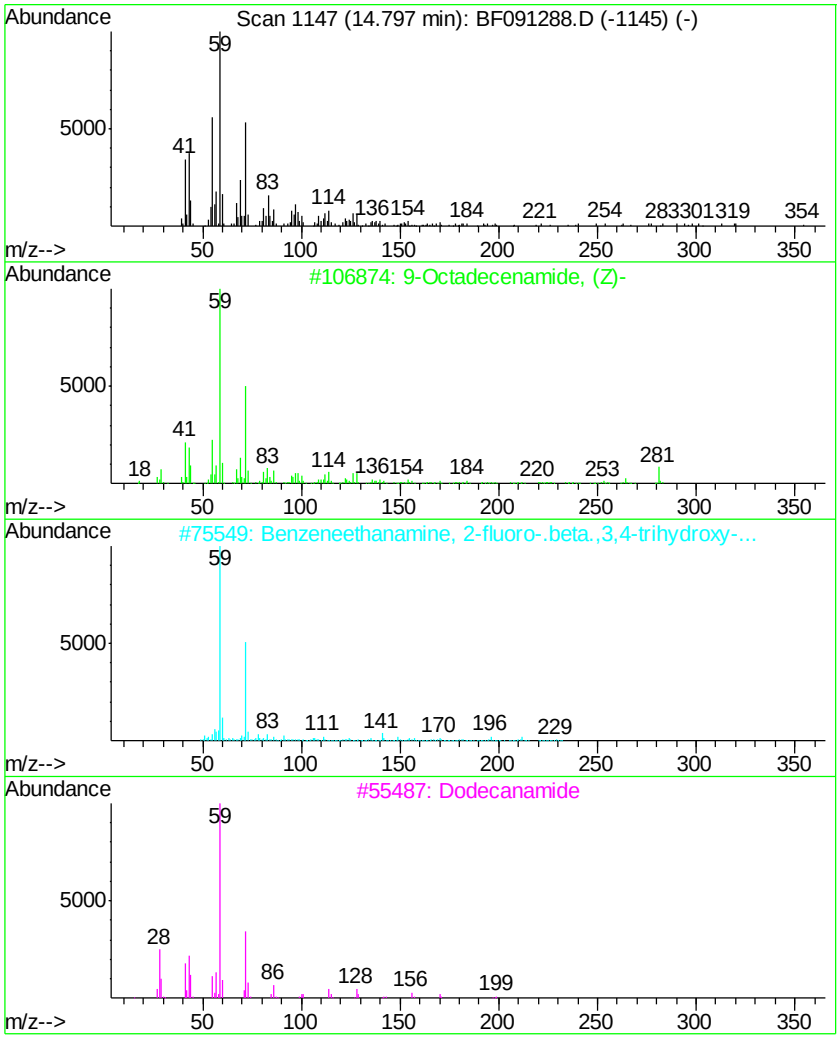
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

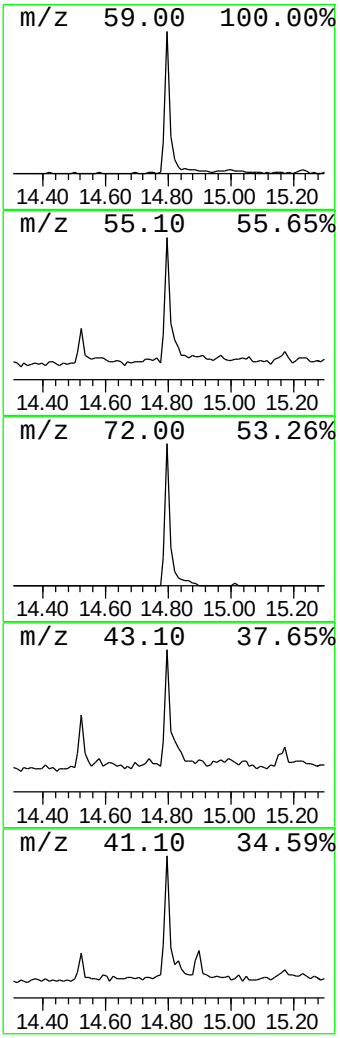
****

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.26 ng	265643	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3	Dodecanamide	199	C12H25NO	001120-16-7	62
4	Hexadecanamide	255	C16H33NO	000629-54-9	59
5	trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	1.77	95.8	ng	6197480	1	6.88	1294300	20.0
Propane, 1,1-dime...	2.18	3.1	ng	201797	1	6.88	1294300	20.0
2-Pentanone, 4-hy...	5.07	33.3	ng	2157070	1	6.88	1294300	20.0
unknown6.65	6.65	82.9	ng	5364440	1	6.88	1294300	20.0
n-Hexadecanoic acid	11.94	5.8	ng	508652	4	11.40	1742210	20.0
Octadecanoic acid	12.72	4.2	ng	368878	4	11.40	1742210	20.0
1-Docosene	13.88	4.1	ng	267606	5	14.03	1307510	20.0
1,2:3,4-Dibenzopy...	14.16	4.5	ng	294572	5	14.03	1307510	20.0
9-Octadecenamide,...	14.80	4.3	ng	265643	6	15.47	1247320	20.0