LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088607.D
Acq On : 2 Jul 2016 7:26
Operator : UM/SJ
Sample : H3831-14
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22-COMP

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-BF063016.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	4	9	11	rVB	5138865	8602964	100.00%	19.396%
2	1.735	11	13	23	rVB	548987	869727	10.11%	1.961%
3	1.861	23	24	41	rVB	2219170	4410847	51.27%	9.945%
4	2.067	41	42	87	rVB	126893	620352	7.21%	1.399%
5	4.993	295	298	304	rVB	250846	373896	4.35%	0.843%
6	5.416	331	335	337	rBV	2400232	3620658	42.09%	8.163%
7	6.444	421	425	427	rBV	2926320	3396319	39.48%	7.657%
8	6.582	433	437	439	rBV	2715452	3677276	42.74%	8.291%
9	6.810	454	457	459	rBV	838690	810258	9.42%	1.827%
10	6.970	468	471	473	rVB	2291353	2899924	33.71%	6.538%
11	7.370	503	506	508	rBV	1938662	2099762	24.41%	4.734%
12	8.090	566	569	571	rVB	1209221	1034254	12.02%	2.332%
13	9.176	660	664	666	rBV	2899195	3847124	44.72%	8.674%
14	9.565	695	698	700	rBV	207883	232505	2.70%	0.524%
15	9.839	720	722	725	rVB	1083712	977025	11.36%	2.203%
16	10.628	788	791	793	rBV	1807486	1758868	20.44%	3.966%
17	11.314	849	851	854	rVB2	726527	775485	9.01%	1.748%
18	11.851	896	898	901	rBV	77568	95304	1.11%	0.215%
19	12.902	987	990	993	rBV	2509383	2490007	28.94%	5.614%
20	13.828	1068	1071	1079	rBV	45081	107101	1.24%	0.241%
21	13.942	1079	1081	1083	rBV	825251	726223	8.44%	1.637%
22	14.800	1153	1156	1158	rBV	361346	369828	4.30%	0.834%
23	15.337	1201	1203	1206	rBV	367245	557839	6.48%	1.258%

Sum of corrected areas: 44353546

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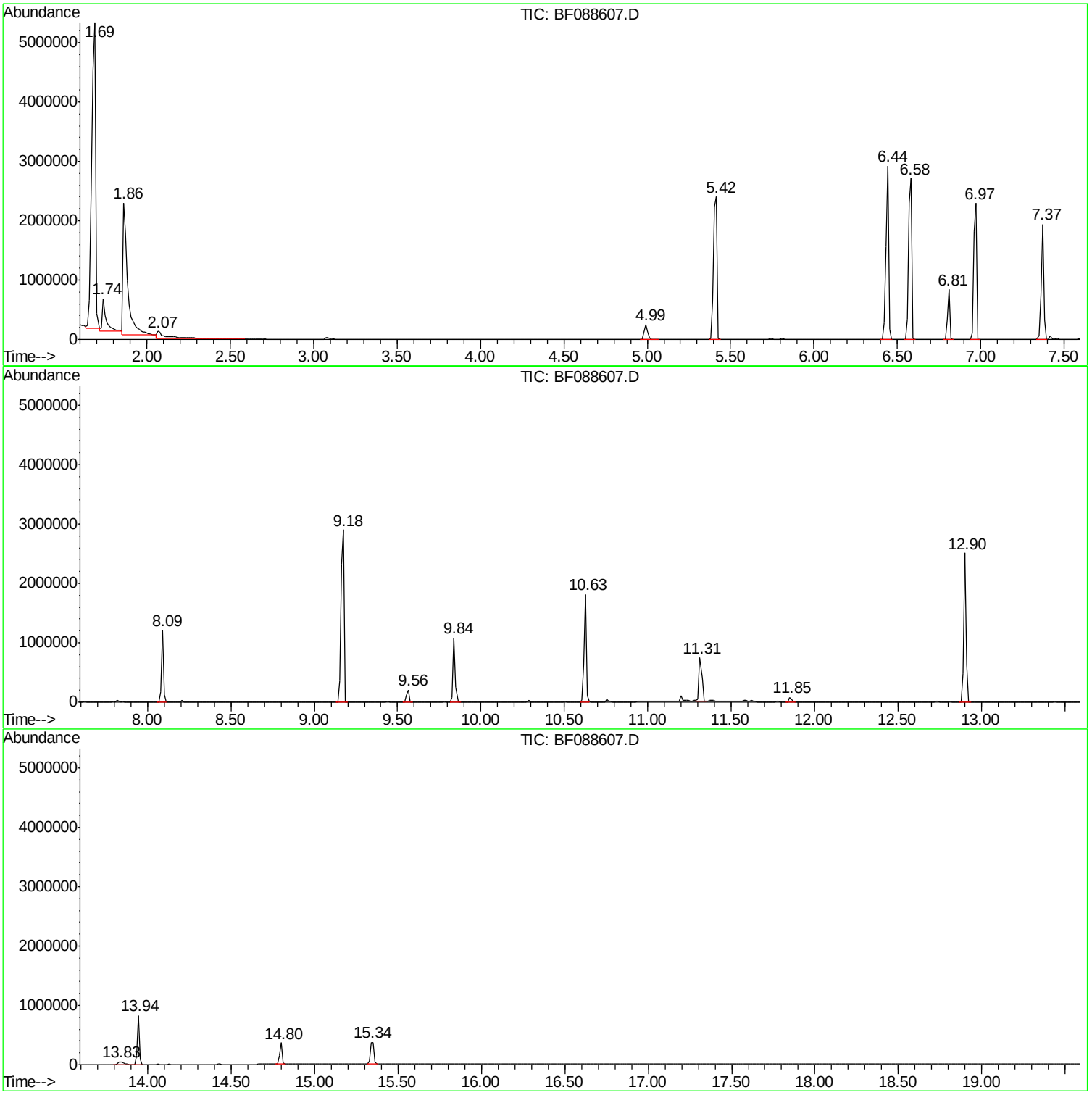
Instrument :
BNA_F
ClientSampleId :
SB-22-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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

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Operator : UM/SJ
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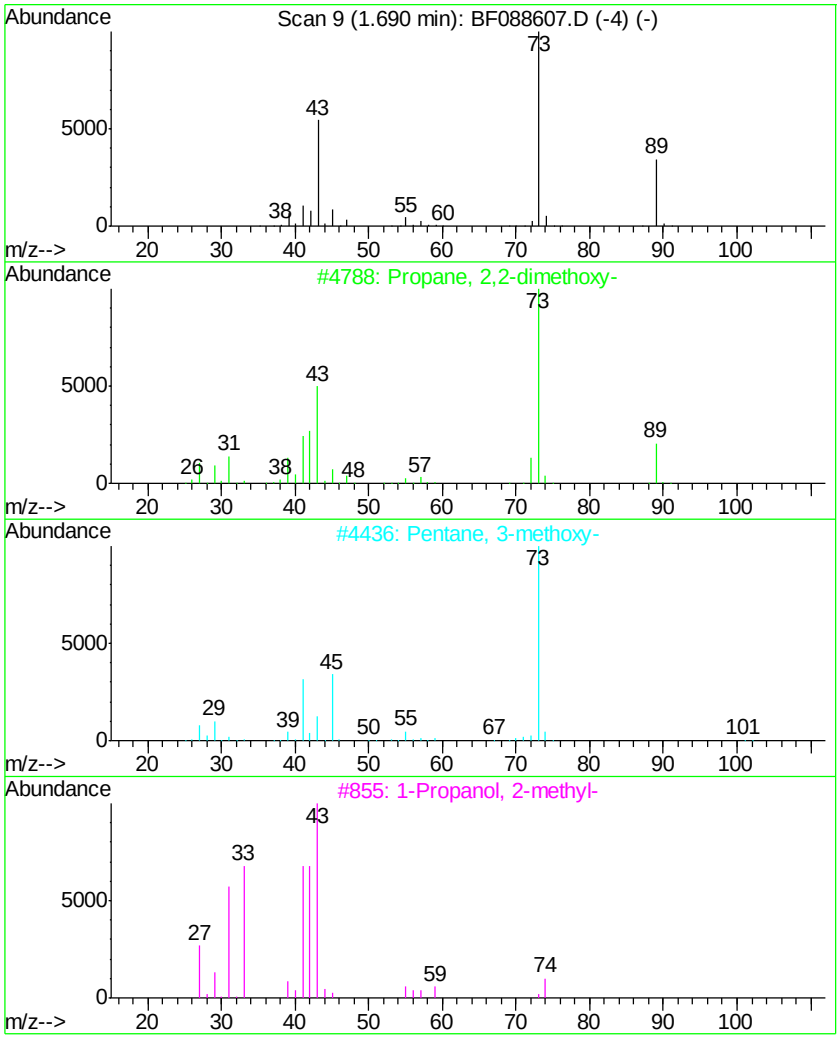
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

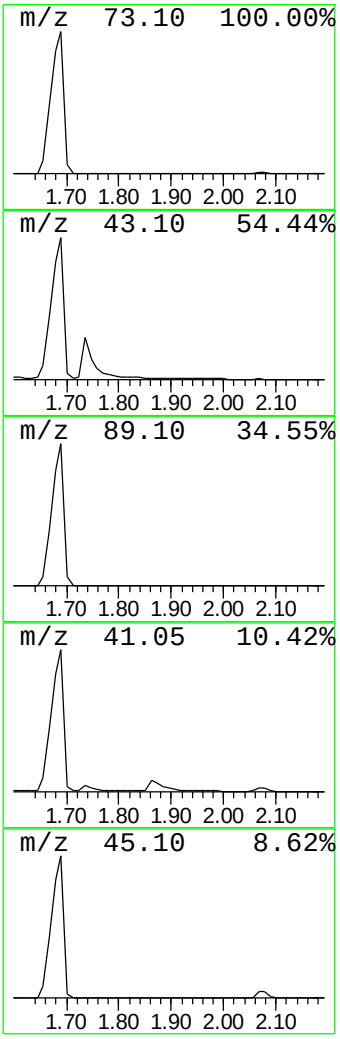
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	212.35 ng	8602960	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Acq On : 2 Jul 2016 7:26
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Sample : H3831-14
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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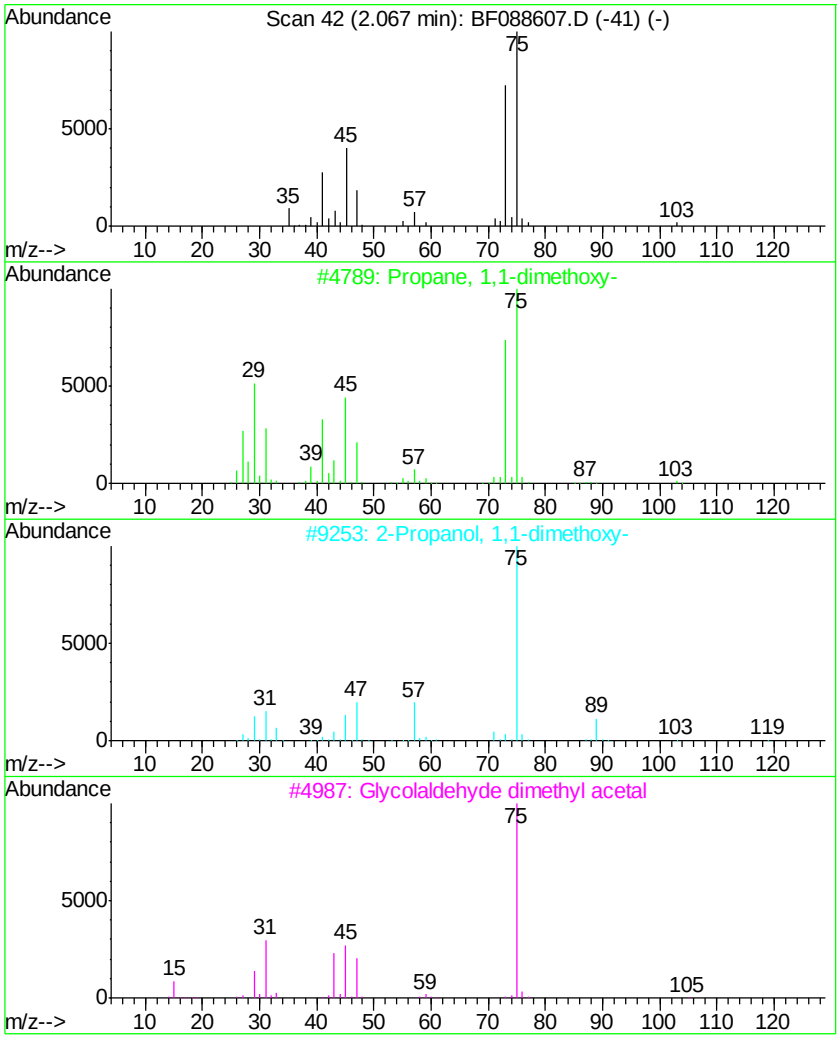
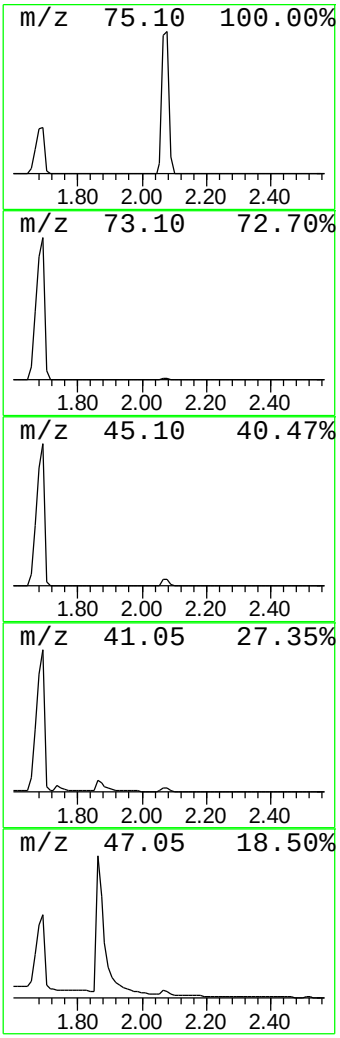
Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	15.31 ng	620352	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
4	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
5	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088607.D
Acq On : 2 Jul 2016 7:26
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Sample : H3831-14
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

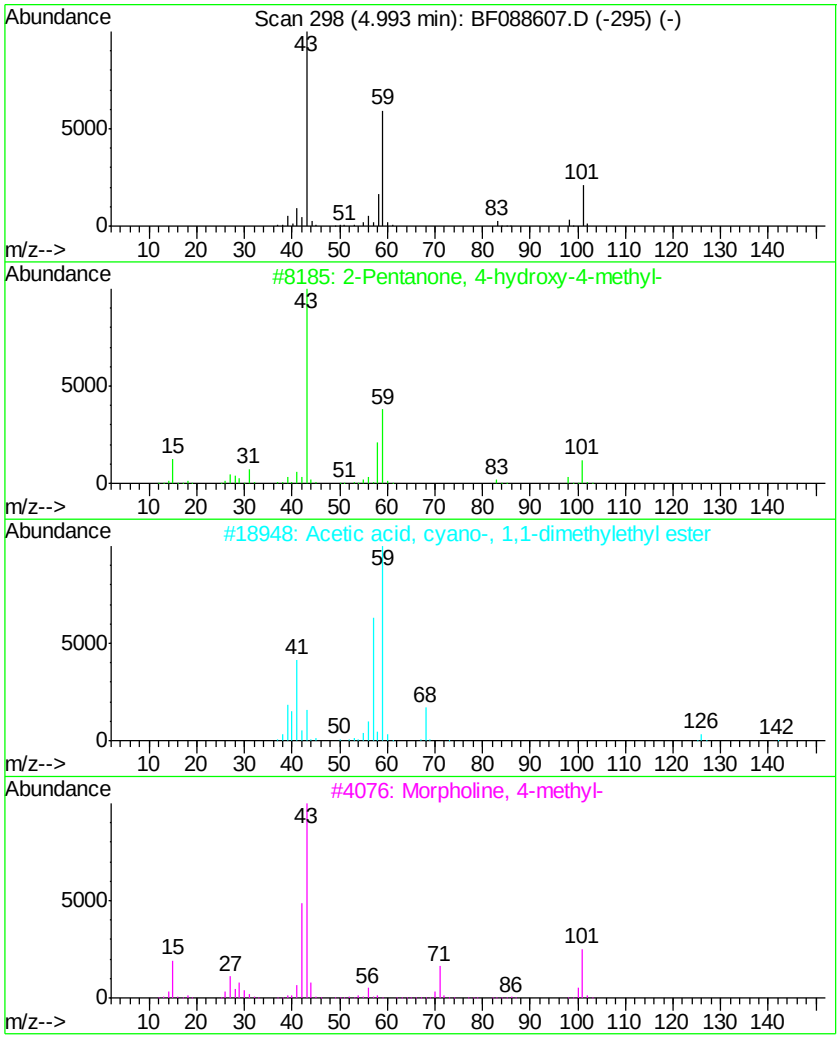
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

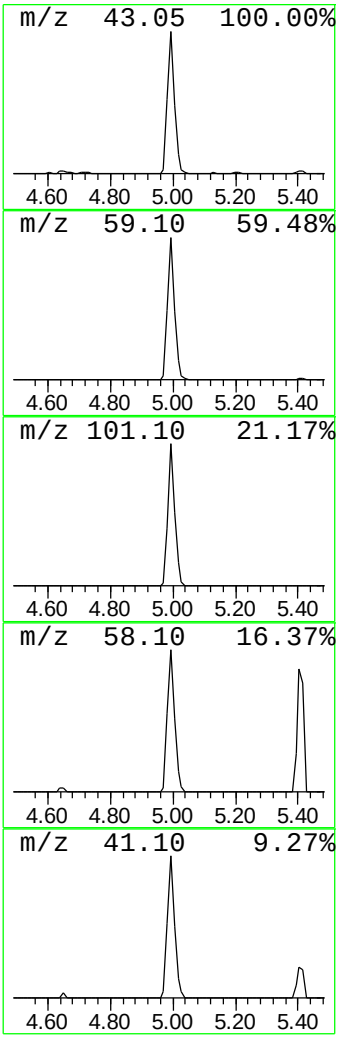
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	9.23 ng	373896	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





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Operator : UM/SJ
Sample : H3831-14
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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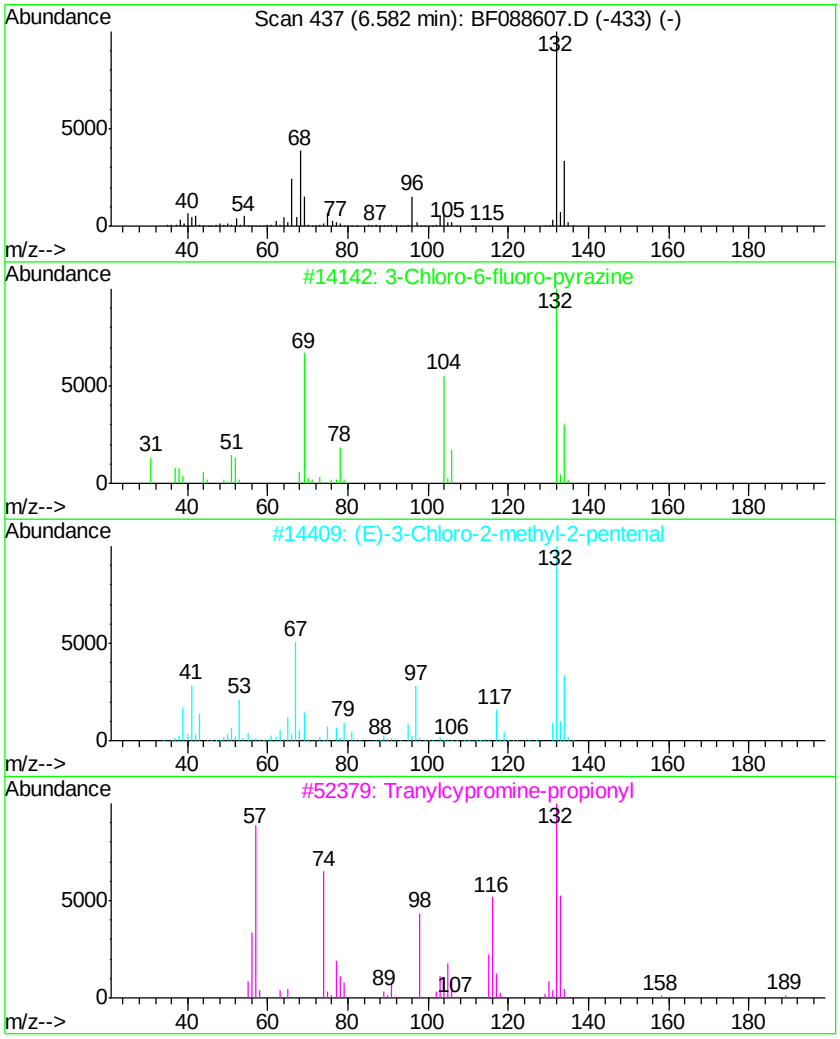
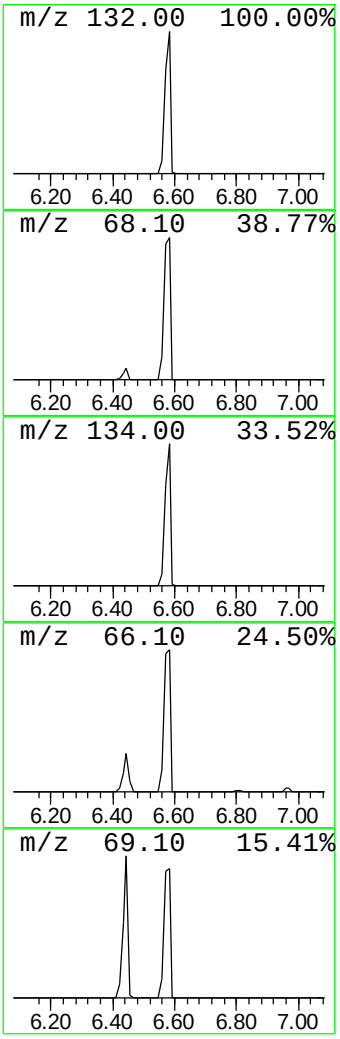
Peak Number 6 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	90.77 ng	3677280	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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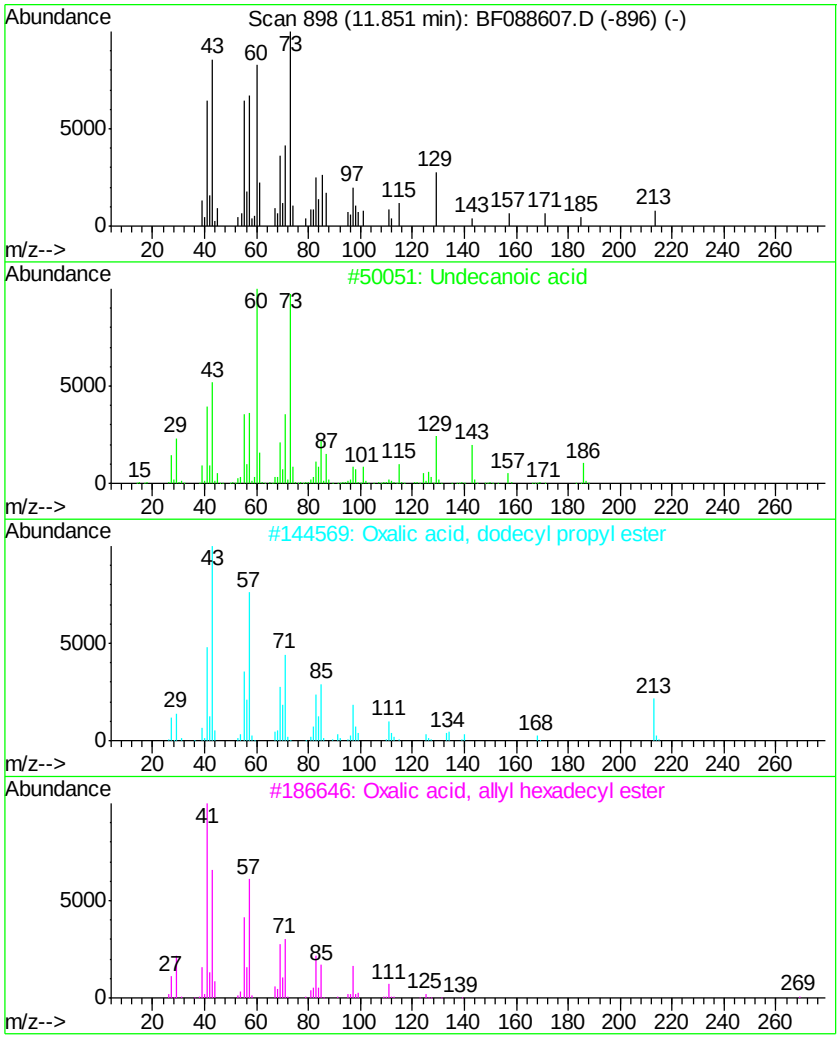
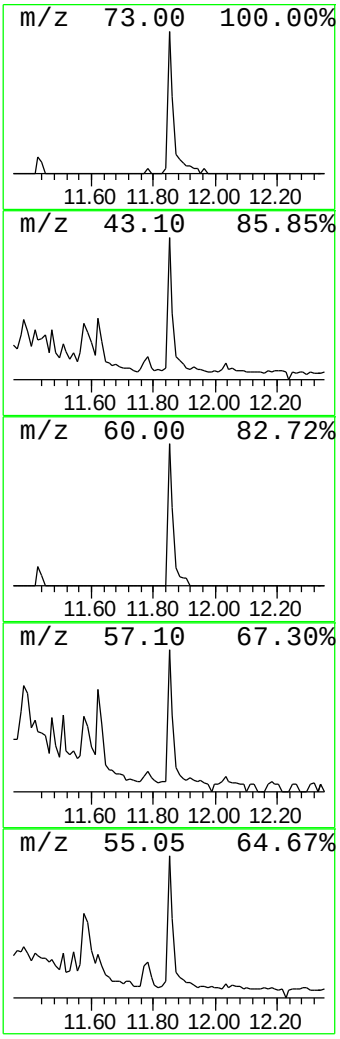
Peak Number 8 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.46 ng	95304	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86
2	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	38
3	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	30
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	25





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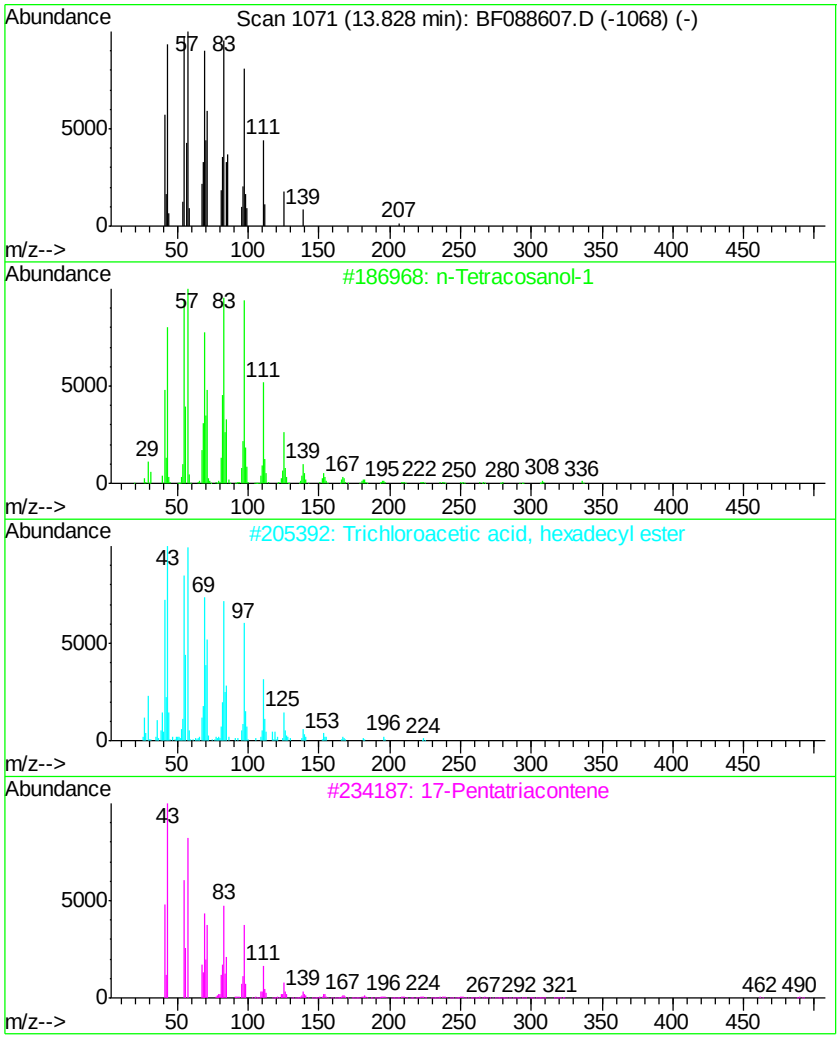
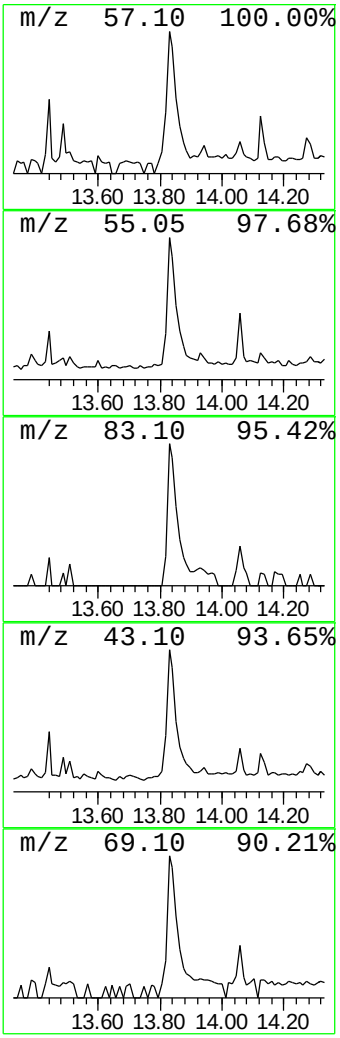
Peak Number 9 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.95 ng	107101	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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TIC Library : C:\Database\NIST11.L
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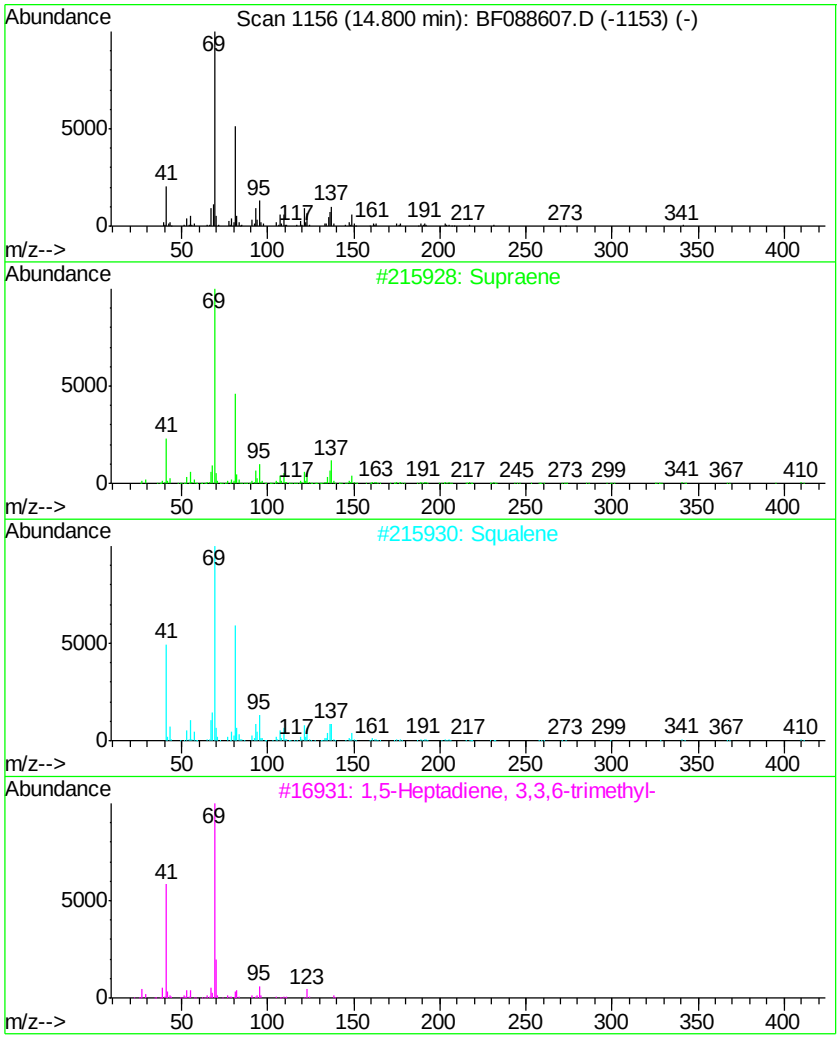
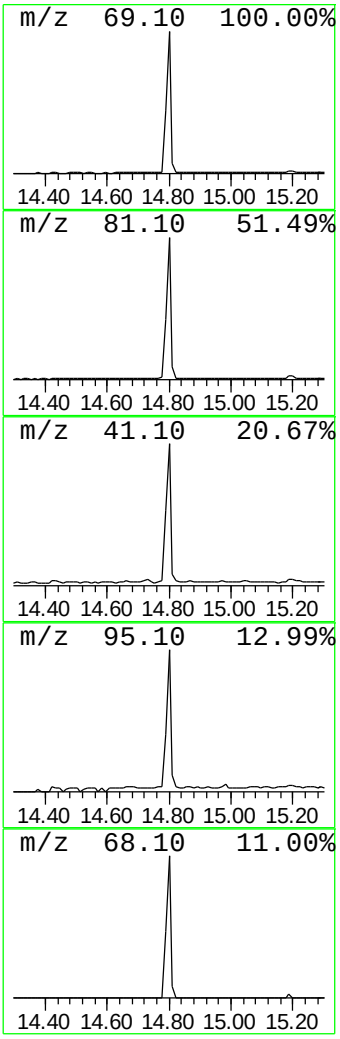
Peak Number 10 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	13.26 ng	369828	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47





Tentatively Identified Compound (LSC) summary

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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, 2,2-dime...	1.69	212.3	ng	8602960	1	6.81	810258	20.0
Propane, 1,1-dime...	2.07	15.3	ng	620352	1	6.81	810258	20.0
2-Pentanone, 4-hy...	4.99	9.2	ng	373896	1	6.81	810258	20.0
unknown6.58	6.58	90.8	ng	3677280	1	6.81	810258	20.0
Undecanoic acid	11.85	2.5	ng	95304	4	11.31	775485	20.0
n-Tetracosanol-1	13.83	3.0	ng	107101	5	13.94	726223	20.0
Supraene	14.80	13.3	ng	369828	6	15.35	557839	20.0