LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087850.D
Acq On : 9 Jun 2016 14:07
Operator : UM/SJ
Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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	1.656	3	6	9	rVB	3281220	5277667	100.00%	15.154%
2	1.747	13	14	24	rVB	368049	592665	11.23%	1.702%
3	1.873	24	25	39	rVB	1675966	3390160	64.24%	9.735%
4	2.056	39	41	52	rVB2	79984	187911	3.56%	0.540%
5	2.193	52	53	71	rVB2	25777	99062	1.88%	0.284%
6	4.993	295	298	306	rVB	269744	378409	7.17%	1.087%
7	5.416	332	335	337	rBV	2258217	2353476	44.59%	6.758%
8	6.456	423	426	428	rBV	2325700	2546569	48.25%	7.312%
9	6.582	435	437	440	rBV	1877158	2565590	48.61%	7.367%
10	6.822	455	458	460	rBV	770075	728144	13.80%	2.091%
11	6.970	469	471	474	rVB	1531206	2028628	38.44%	5.825%
12	7.382	504	507	510	rBV	1482920	1486393	28.16%	4.268%
13	8.102	568	570	573	rBV	1109702	965665	18.30%	2.773%
14	9.176	661	664	667	rBV	2638101	2832636	53.67%	8.134%
15	9.565	696	698	701	rBV	231716	319758	6.06%	0.918%
16	9.793	716	718	721	rBV	62481	56771	1.08%	0.163%
17	9.851	721	723	726	rVB	1281588	1111488	21.06%	3.192%
18	10.285	757	761	763	rBV	74631	92398	1.75%	0.265%
19	10.514	777	781	784	rBV	28745	54458	1.03%	0.156%
20	10.639	789	792	794	rBV	1801832	1864721	35.33%	5.354%
21	10.765	801	803	807	rBV	80439	133806	2.54%	0.384%
22	11.211	840	842	843	rBV	45487	55480	1.05%	0.159%
23	11.325	850	852	855	rBV	1066072	1071597	20.30%	3.077%
24	12.742	973	976	978	rBV	136796	119540	2.27%	0.343%
25	12.914	988	991	993	rBV	2654600	2551189	48.34%	7.326%
26	13.440	1035	1037	1039	rBV	80014	82813	1.57%	0.238%
27	13.805	1067	1069	1076	rBV	166632	267943	5.08%	0.769%
28	13.954	1079	1082	1084	rBV	879273	833070	15.78%	2.392%
29	14.800	1153	1156	1158	rBV	84664	82157	1.56%	0.236%
30	15.360	1202	1205	1207	rBV	604024	695734	13.18%	1.998%

Sum of corrected areas: 34825898

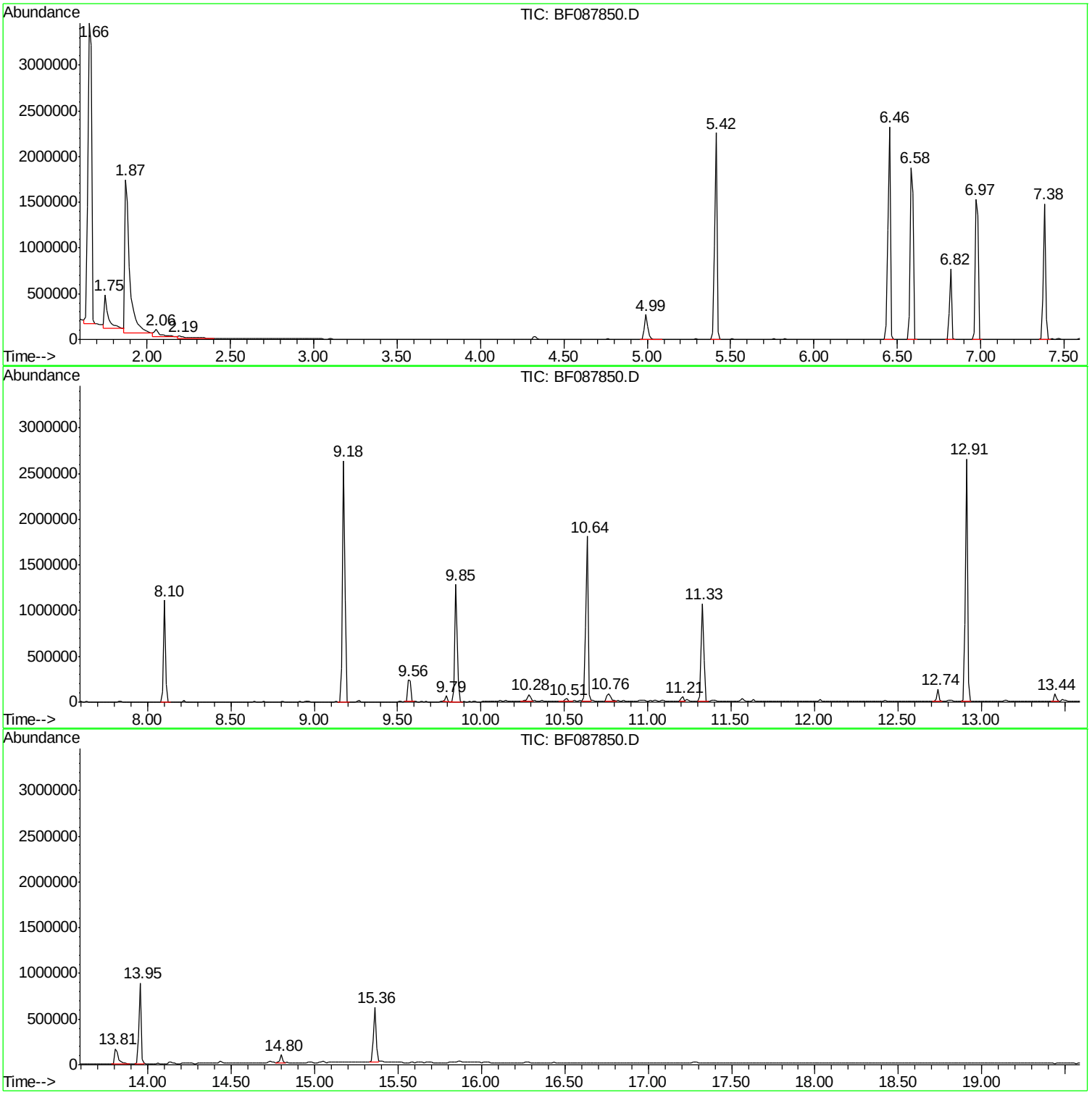
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087850.D
Acq On : 9 Jun 2016 14:07
Operator : UM/SJ
Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1300-04-SW-06072016

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087850.D
Acq On : 9 Jun 2016 14:07
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ClientSampleId : 1300-04-SW-06072016

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

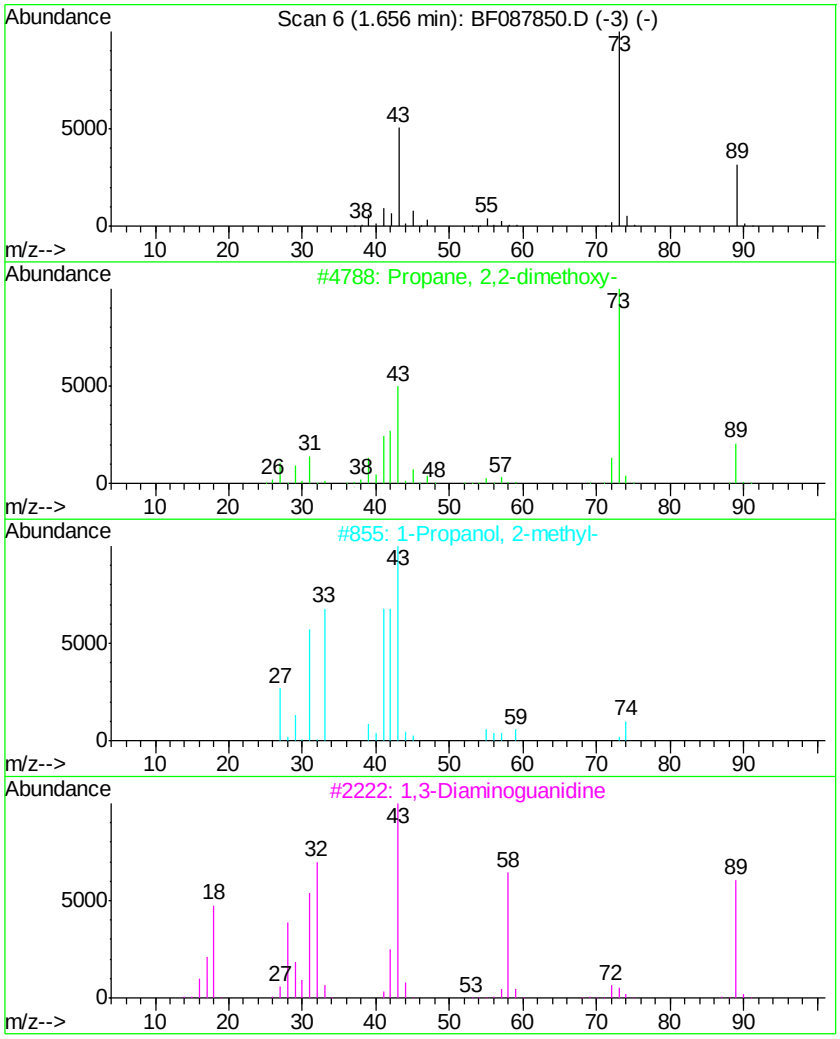
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

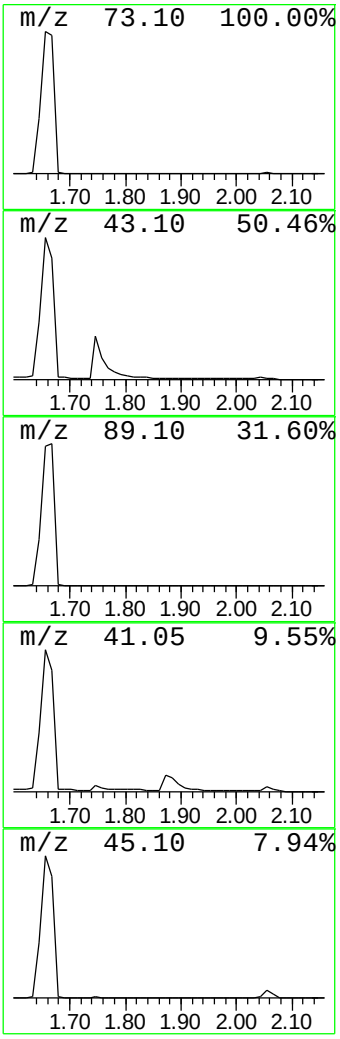
****

Peak Number 1 unknown1.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	144.96 ng	5277670	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Sample : H3477-04
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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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

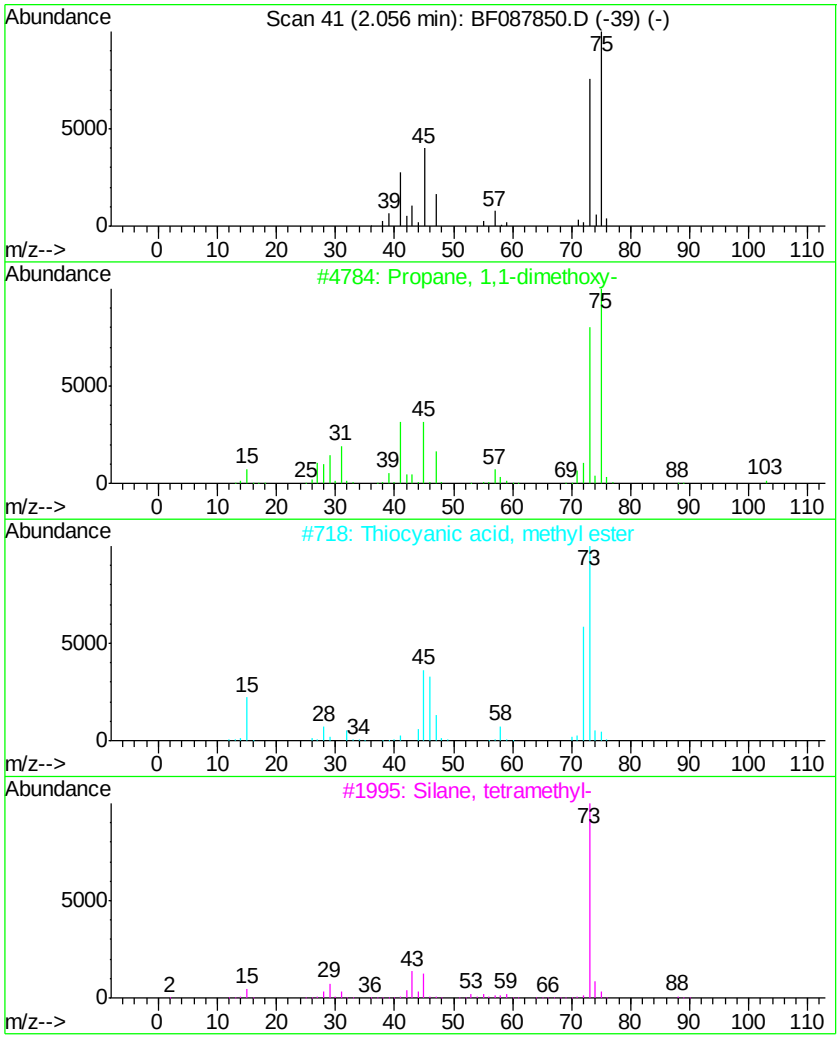
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

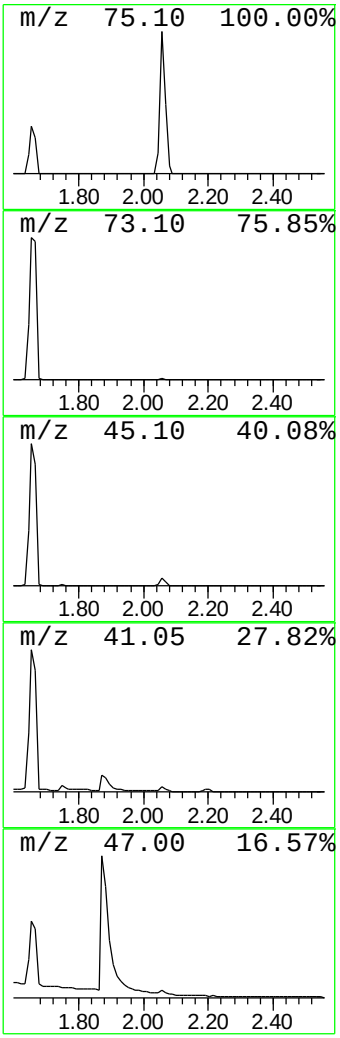
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	5.16 ng	187911	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1300-04-SW-06072016

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

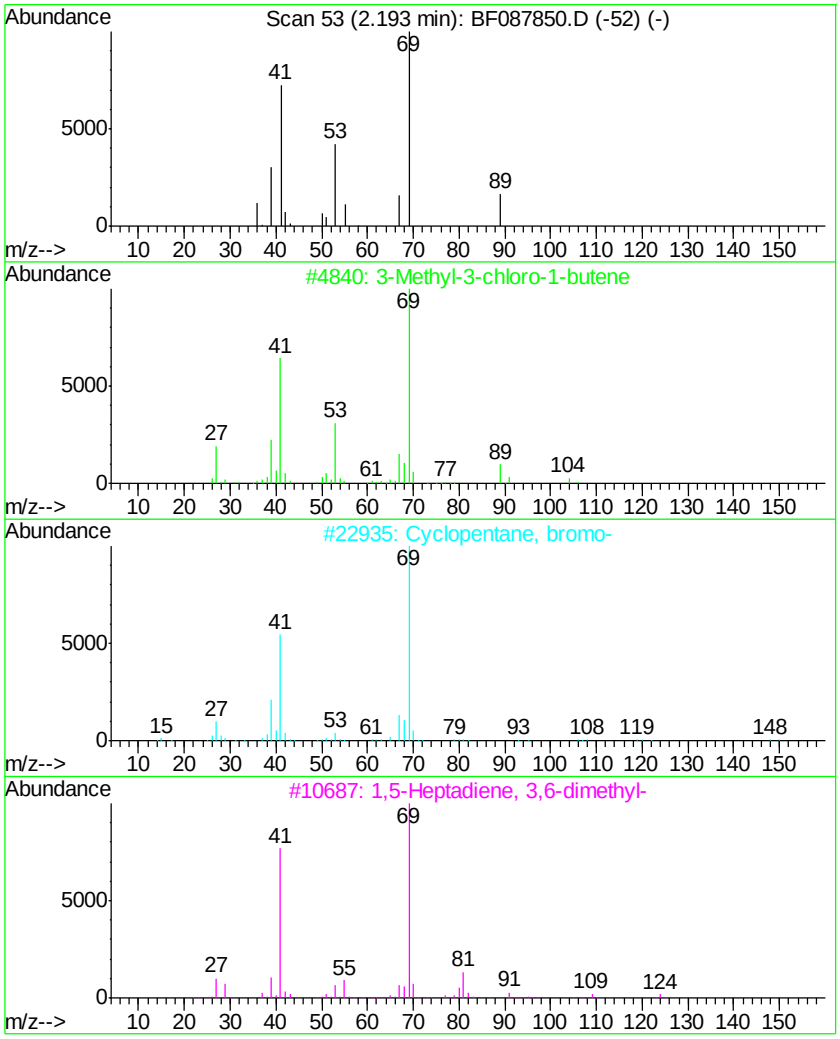
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

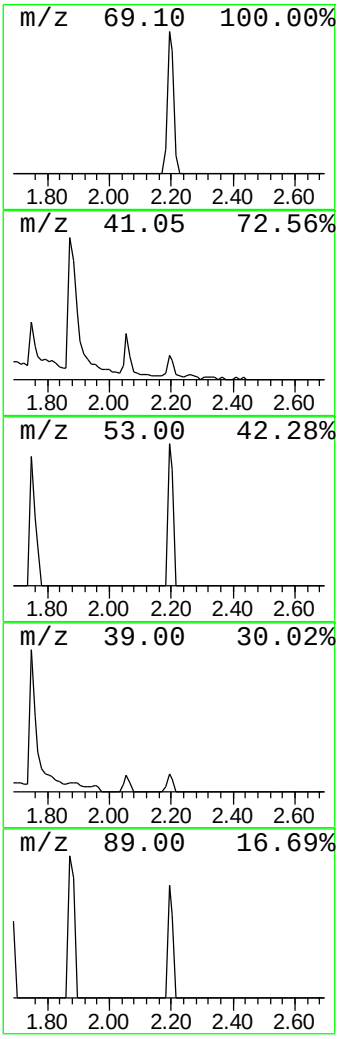
****

Peak Number 5 unknown2.19 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	2.72 ng	99062	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	17
2	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	9
3	1,5-Heptadiene, 3,6-dimethyl-	124	C9H16	034891-10-6	4
4	2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	3
5	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	3





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087850.D
Acq On : 9 Jun 2016 14:07
Operator : UM/SJ
Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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

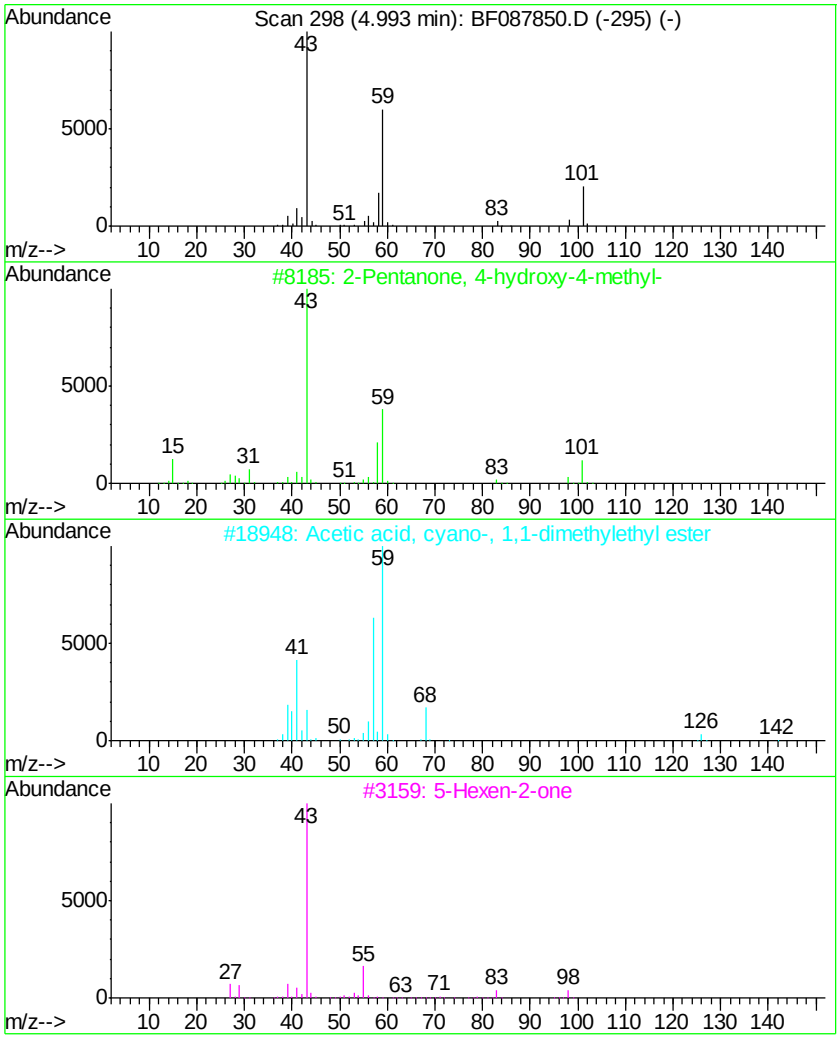
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

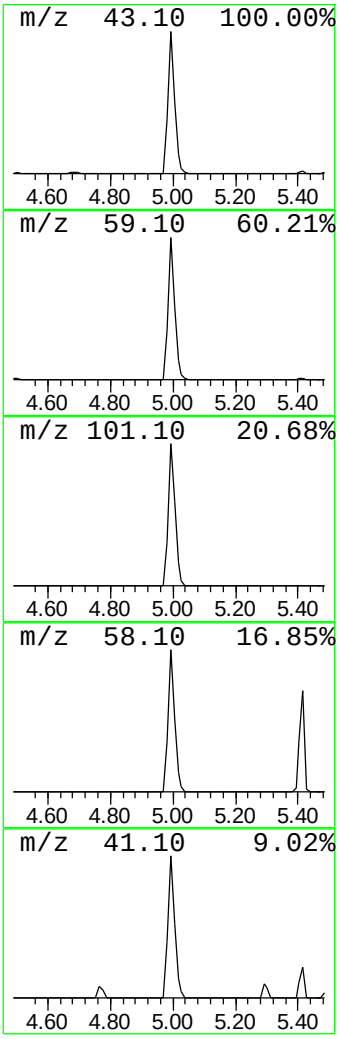
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	10.39 ng	378409	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF087850.D
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Operator : UM/SJ
Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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

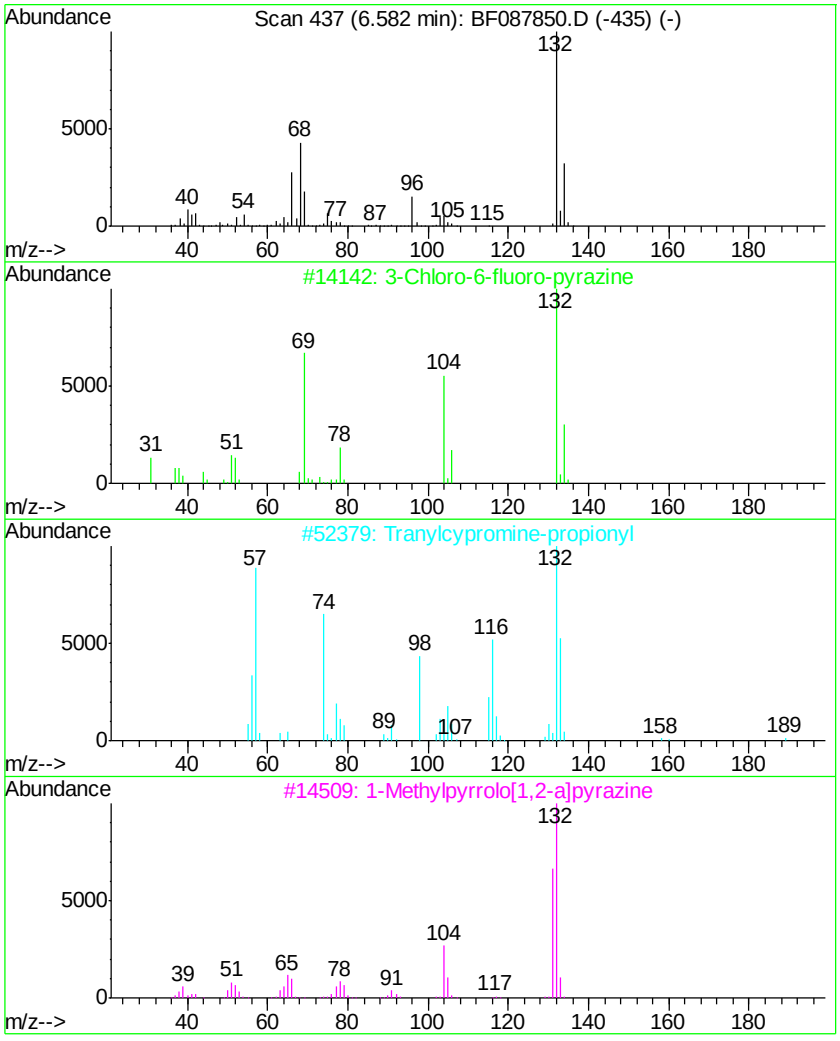
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

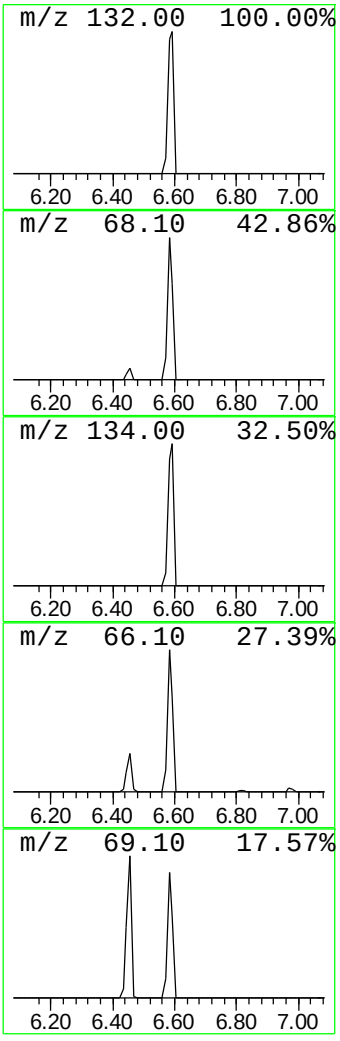
****

Peak Number 7 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	70.47 ng	2565590	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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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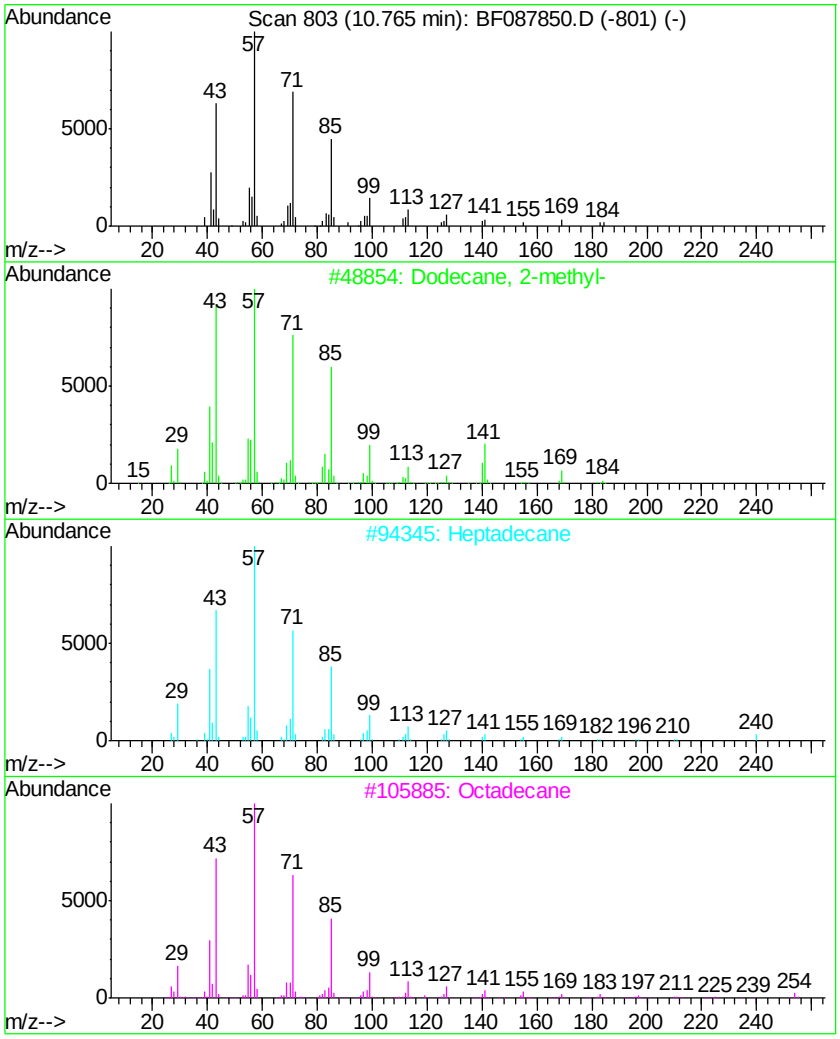
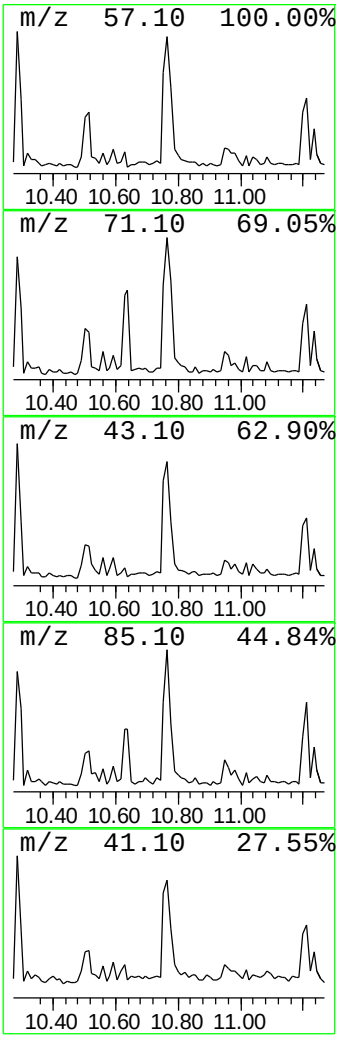
****

Peak Number 9 Dodecane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.50 ng	133806	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	93
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91





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

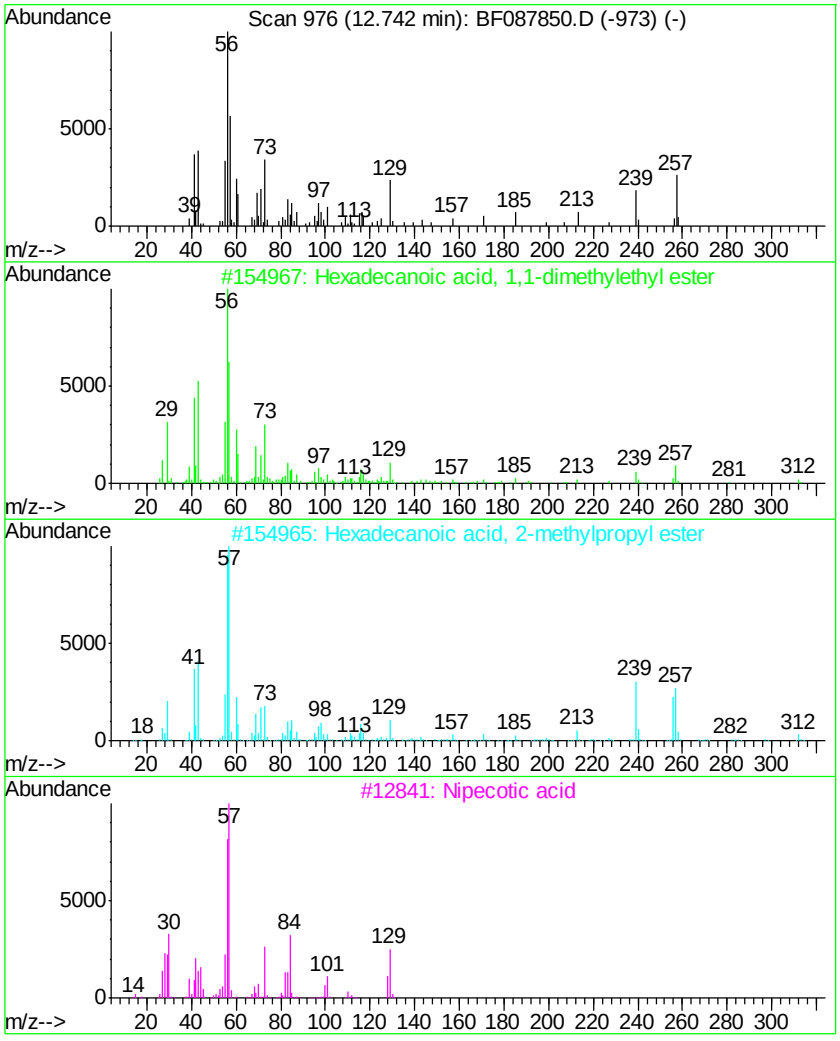
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

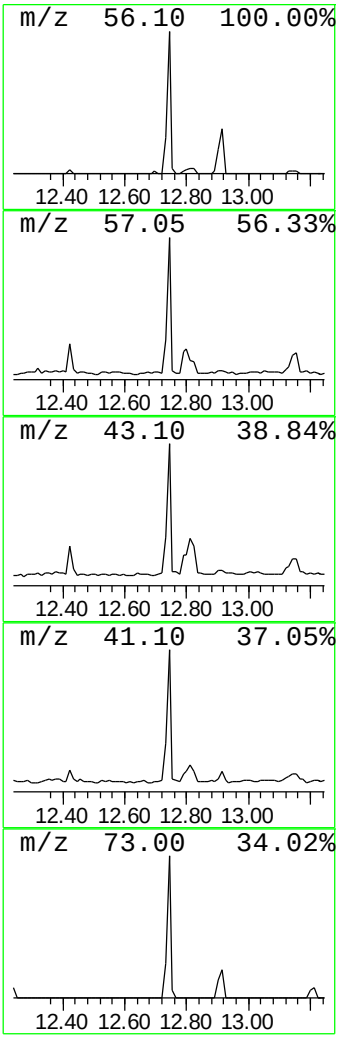
****

Peak Number 10 Hexadecanoic acid, 1,1-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.87 ng	119540	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	72
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	45
5	Cyclohexanamine	99	C6H13N	000108-91-8	30





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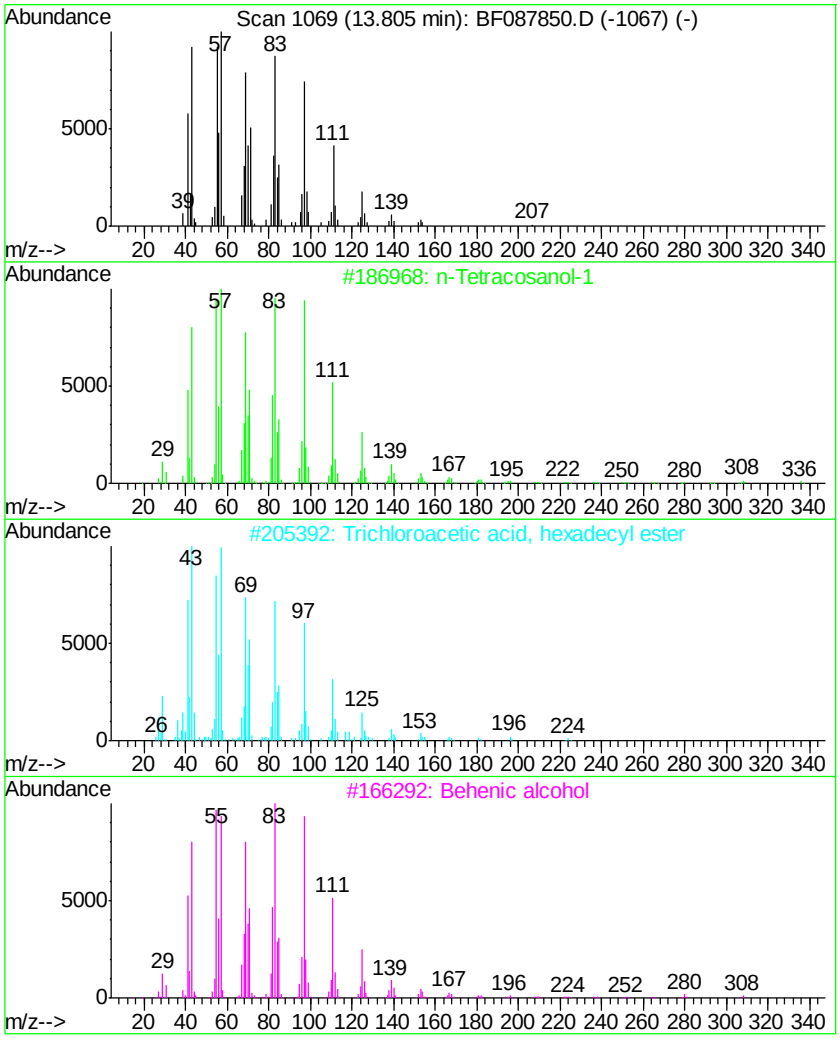
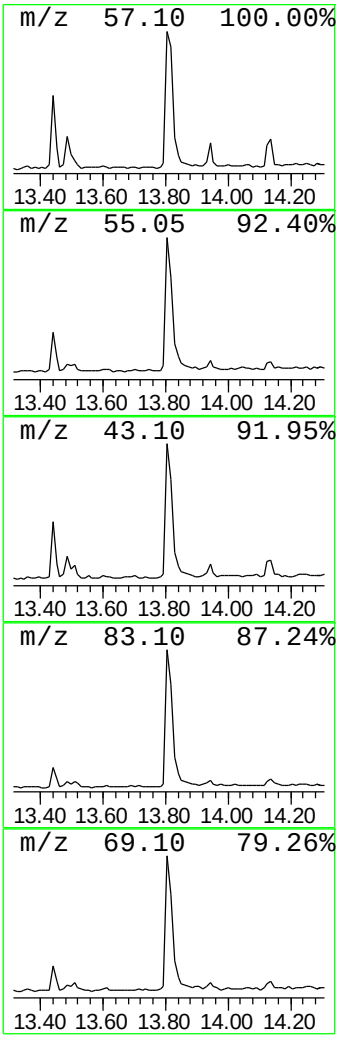
Peak Number 11 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.43 ng	267943	Chrysene-d12	13.95

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	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Data File : BF087850.D
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Operator : UM/SJ
Sample : H3477-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1300-04-SW-06072016

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

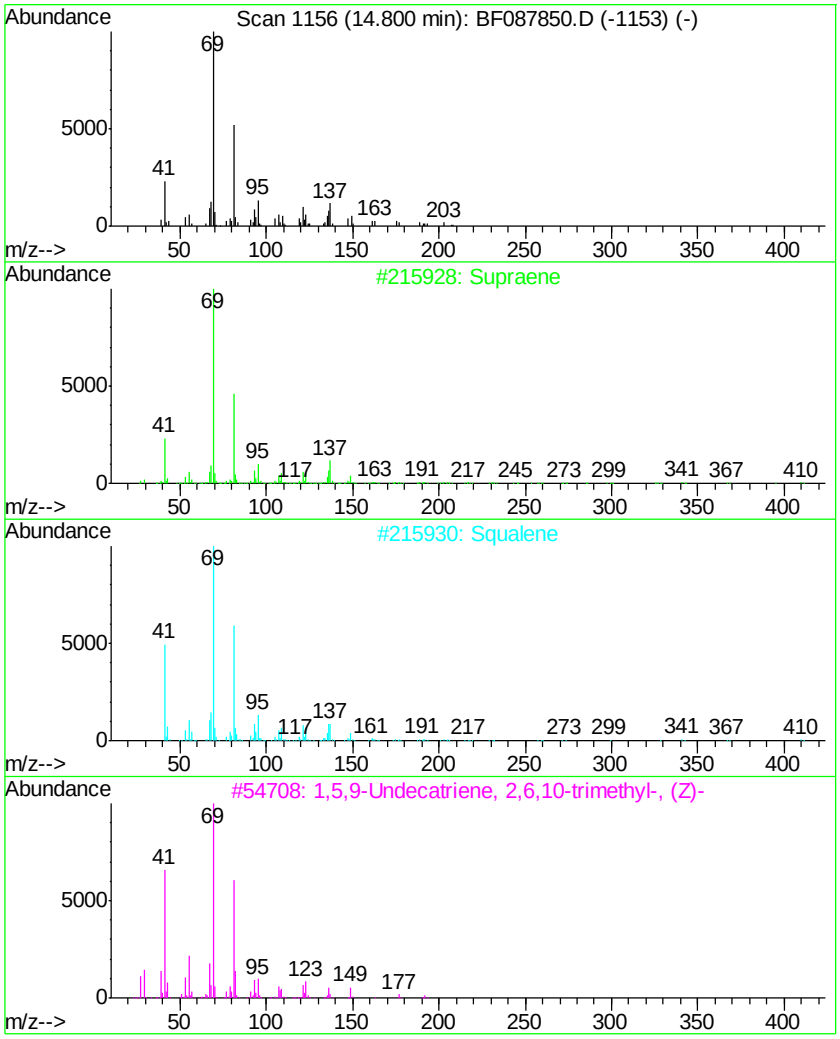
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

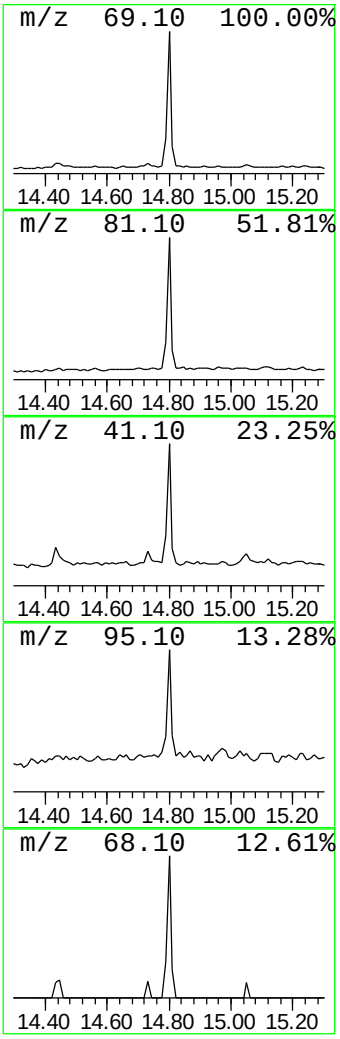
****

Peak Number 12 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.36 ng	82157	Perylene-d12	15.36

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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
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Acq On : 9 Jun 2016 14:07
Operator : UM/SJ
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Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.66	1.66	145.0	ng	5277670	1	6.82	728144	20.0
Propane, 1,1-dime...	2.06	5.2	ng	187911	1	6.82	728144	20.0
unknown2.19	2.19	2.7	ng	99062	1	6.82	728144	20.0
2-Pentanone, 4-hy...	4.99	10.4	ng	378409	1	6.82	728144	20.0
unknown6.58	6.58	70.5	ng	2565590	1	6.82	728144	20.0
Dodecane, 2-methyl-	10.77	2.5	ng	133806	4	11.32	1071600	20.0
Hexadecanoic acid...	12.74	2.9	ng	119540	5	13.95	833070	20.0
n-Tetracosanol-1	13.81	6.4	ng	267943	5	13.95	833070	20.0
Supraene	14.80	2.4	ng	82157	6	15.36	695734	20.0