LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

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-BF050416.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	4.864	242	243	251	rBV	97901	192564	3.02%	0.449%
2	5.310	279	282	300	rBV	1593767	2654745	41.65%	6.193%
3	5.710	312	317	323	rVB2	34318	66896	1.05%	0.156%
4	6.362	371	374	379	rBV	1679035	1743150	27.35%	4.067%
5	6.476	382	384	387	rBV	4582013	4541797	71.26%	10.595%
6	6.704	402	404	406	rBV	912253	1102405	17.30%	2.572%
7	6.853	415	417	420	rBV	3268024	4107247	64.44%	9.582%
8	6.979	425	428	432	rVB2	41594	76641	1.20%	0.179%
9	7.276	451	454	456	rBV	3528851	3853783	60.46%	8.990%
10	7.767	495	497	503	rVB	43556	75446	1.18%	0.176%
11	7.927	508	511	513	rBV2	723690	712094	11.17%	1.661%
12	7.985	514	516	519	rBV	1279750	1416291	22.22%	3.304%
13	9.070	607	611	613	rBV	5587885	6373744	100.00%	14.869%
14	9.676	662	664	667	rBV	95942	89264	1.40%	0.208%
15	9.733	667	669	672	rVV2	1344456	1512264	23.73%	3.528%
16	10.179	705	708	709	rBV2	108659	115707	1.82%	0.270%
17	10.533	736	739	741	rBV2	2779047	3756989	58.94%	8.765%
18	10.648	747	749	754	rVB	134799	156741	2.46%	0.366%
19	11.219	797	799	801	rBV	1403695	1425263	22.36%	3.325%
20	11.756	844	846	856	rBV2	83584	120833	1.90%	0.282%
21	12.442	904	906	912	rBV3	33576	87484	1.37%	0.204%
22	12.545	912	915	920	rBV	68921	115874	1.82%	0.270%
23	12.625	920	922	925	rVB	215619	251335	3.94%	0.586%
24	12.705	928	929	932	rVB	104723	87063	1.37%	0.203%
25	12.808	935	938	940	rBV	4650095	5452340	85.54%	12.720%
26	13.334	982	984	986	rBV	217412	194917	3.06%	0.455%
27	13.379	986	988	989	rBV	83070	86027	1.35%	0.201%
28	13.711	1014	1017	1021	rBV	101735	159026	2.50%	0.371%
29	13.848	1026	1029	1031	rBV	784122	1022607	16.04%	2.386%
30	14.019	1042	1044	1048	rVB	128043	116351	1.83%	0.271%
31	14.317	1068	1070	1073	rBV	81654	125961	1.98%	0.294%
32	14.614	1094	1096	1099	rBV	92998	96995	1.52%	0.226%
33	15.220	1147	1149	1158	rBV	582535	846283	13.28%	1.974%
34	18.477	1430	1434	1439	rBV	43114	129470	2.03%	0.302%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR2-8

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-BF050416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 42865597

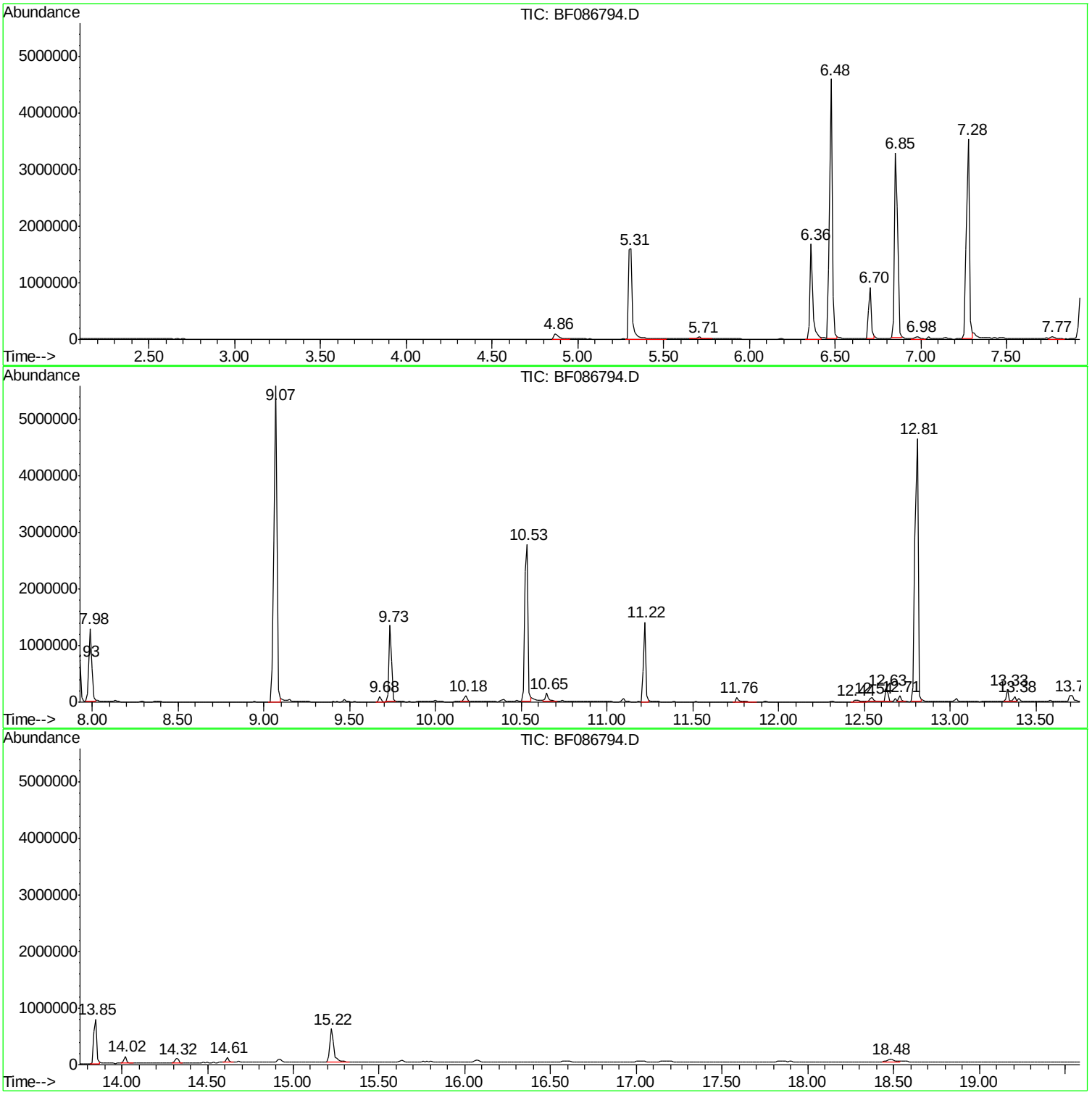
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

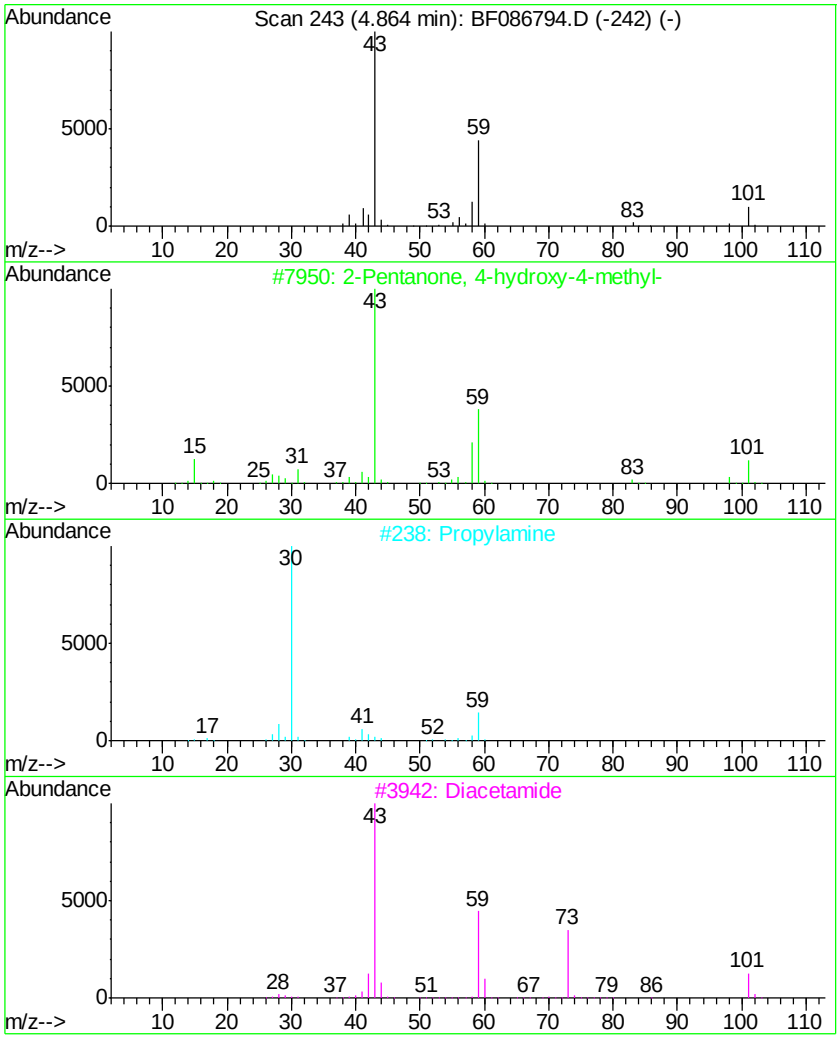
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

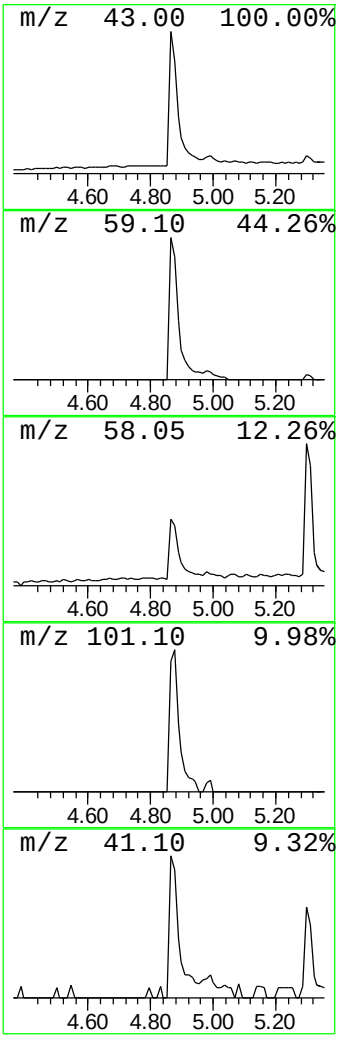
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	6.99 ng	192564	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propylamine	59	C3H9N	000107-10-8	9
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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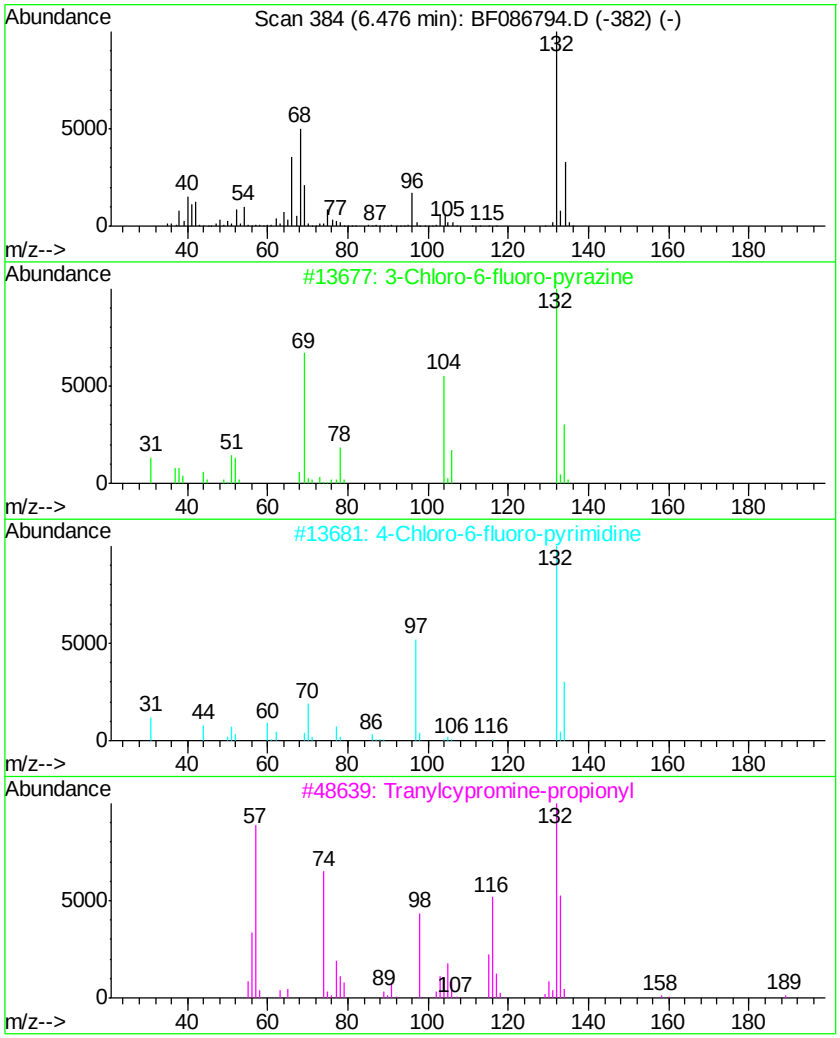
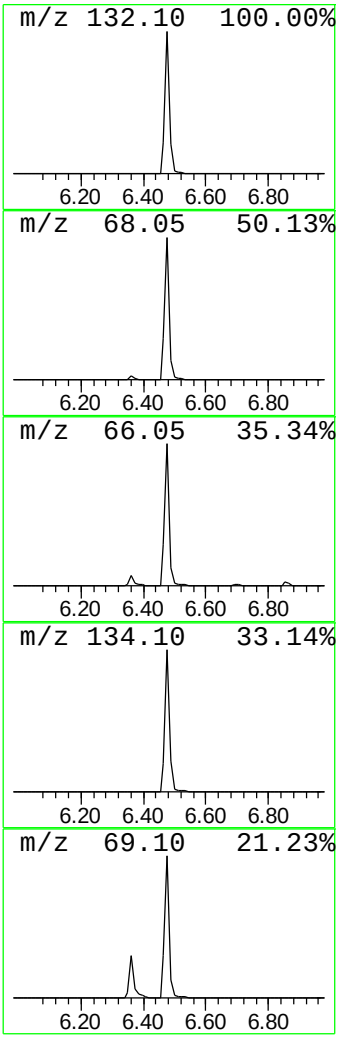
Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	164.80 ng	4541800	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

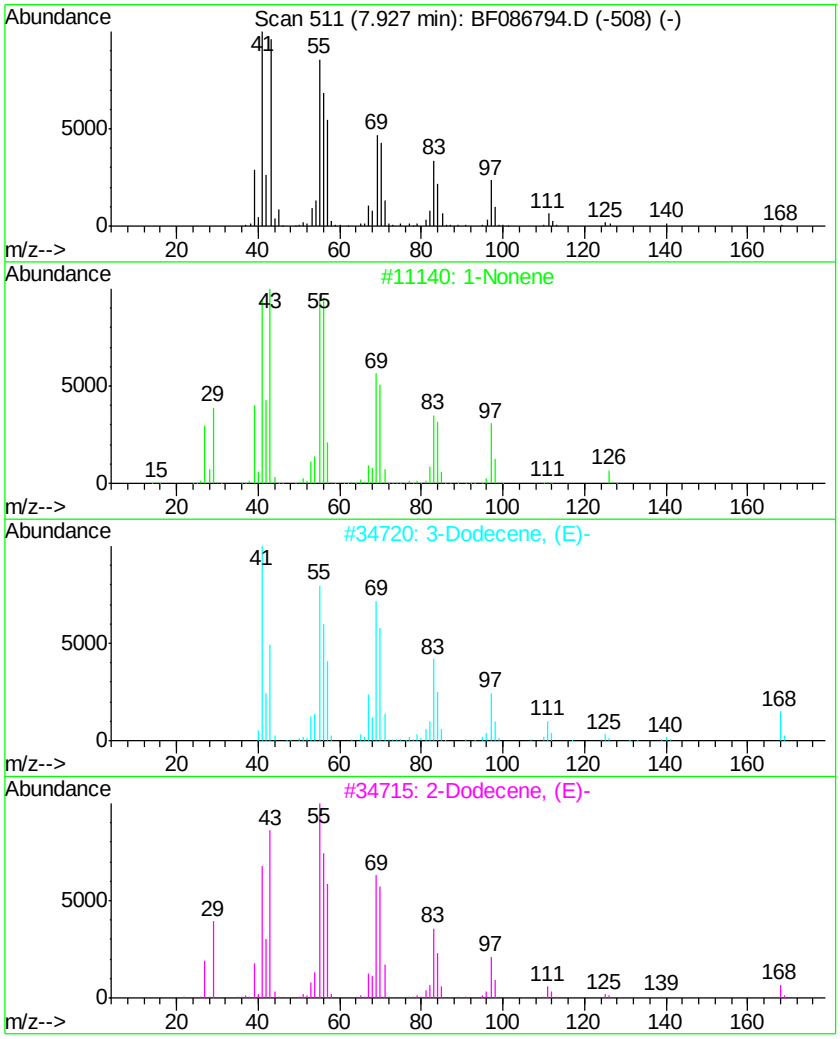
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

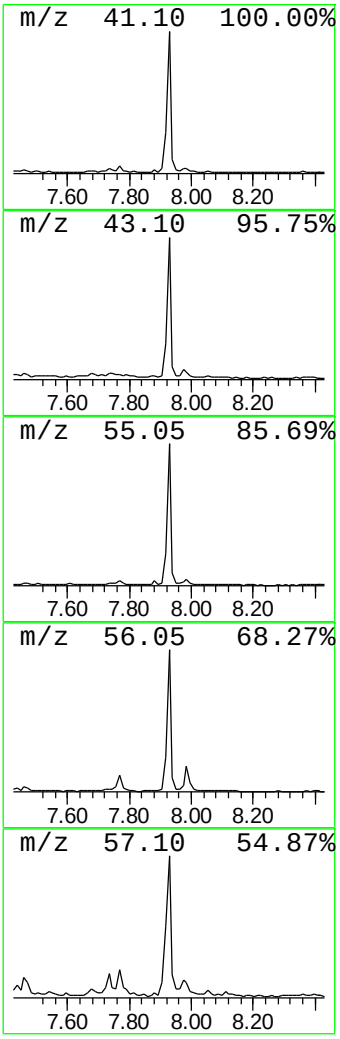
****

Peak Number 4 1-Nonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	20.11 ng	712094	Naphthalene-d8	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene	126	C9H18	000124-11-8	95
2	3-Dodecene, (E)-	168	C12H24	007239-23-8	91
3	2-Dodecene, (E)-	168	C12H24	007206-13-5	91
4	4-Dodecene, (Z)-	168	C12H24	007206-27-1	90
5	5-Dodecene, (Z)-	168	C12H24	007206-28-2	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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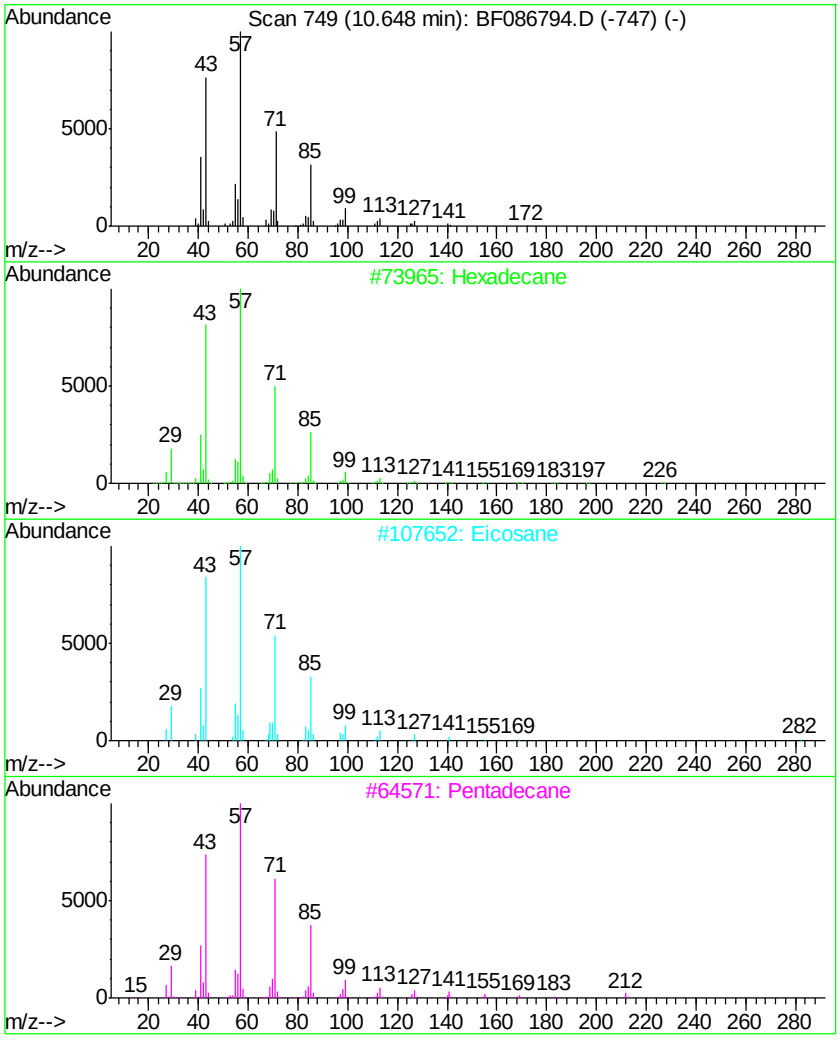
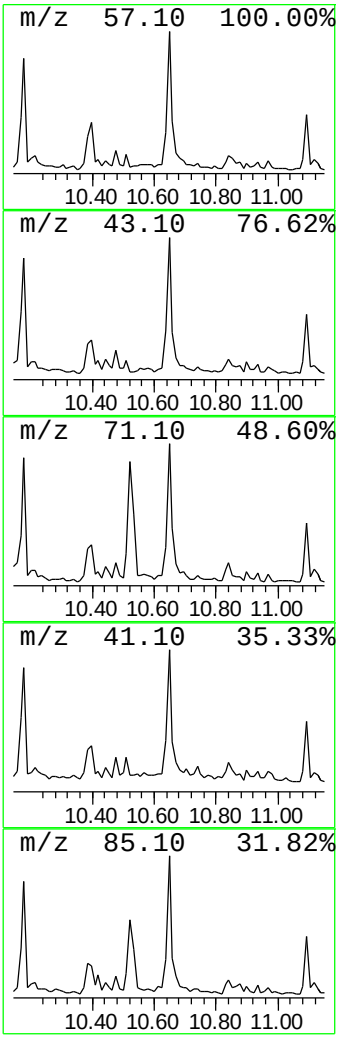
Peak Number 5 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.40 ng	156741	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tridecane	184	C13H28	000629-50-5	86
5	Tetradecane	198	C14H30	000629-59-4	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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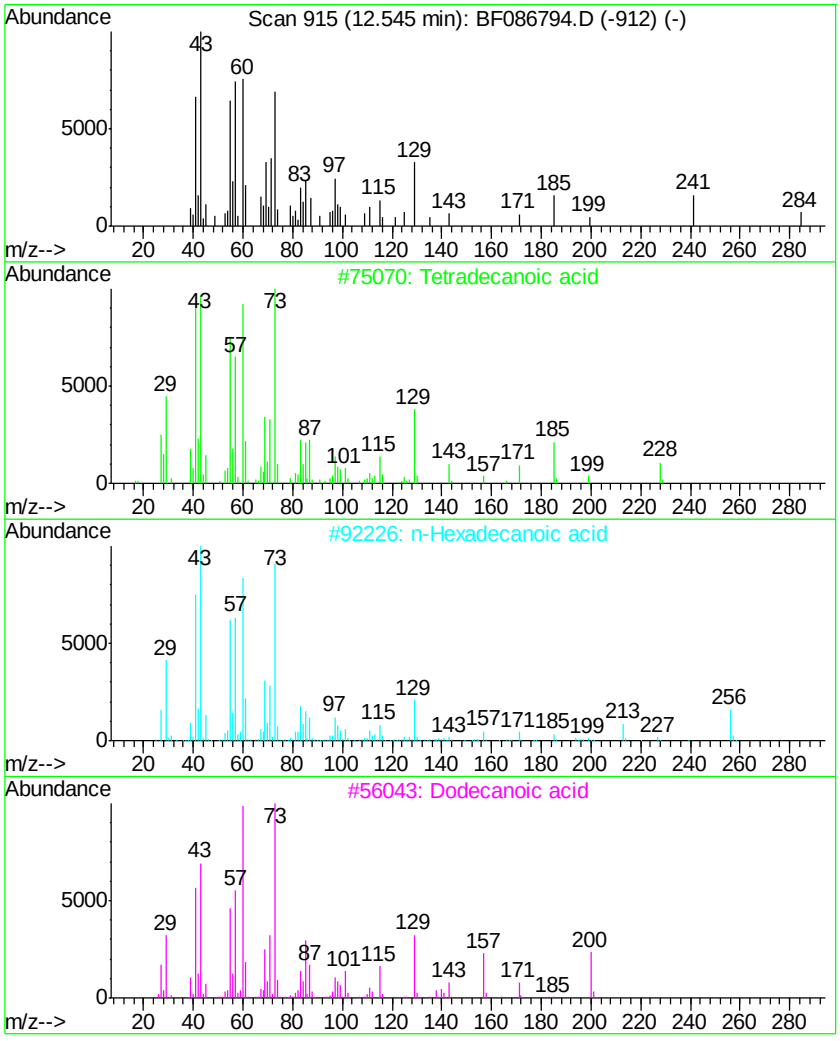
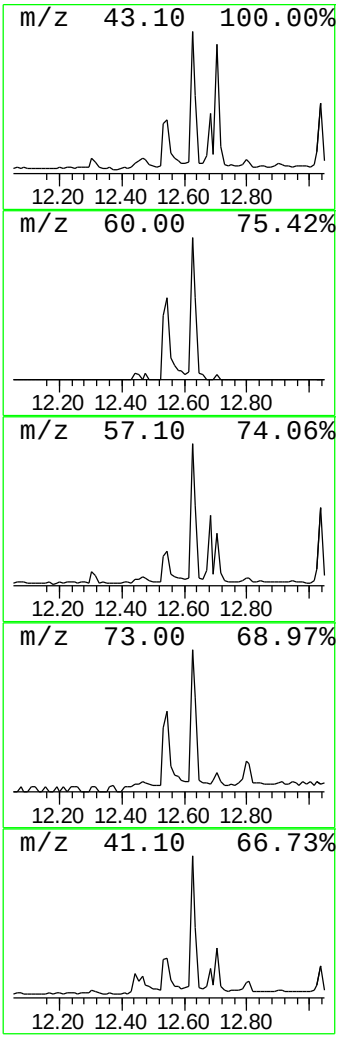
Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	4.53 ng	115874	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

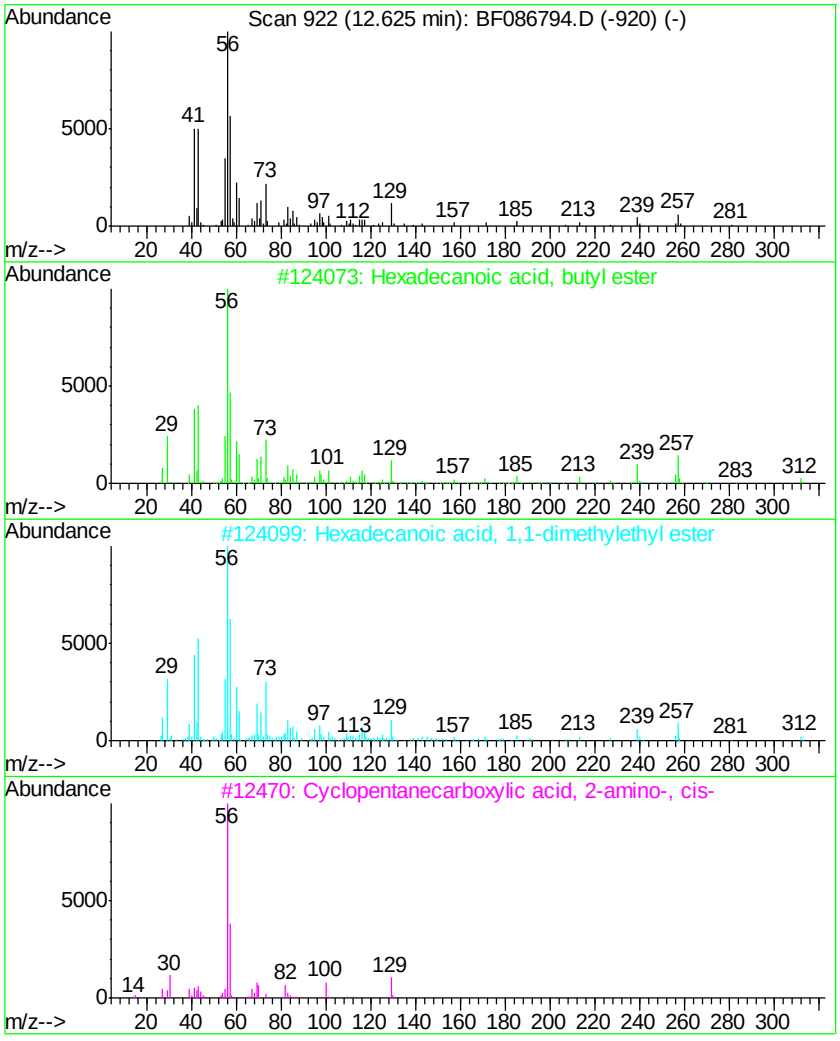
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

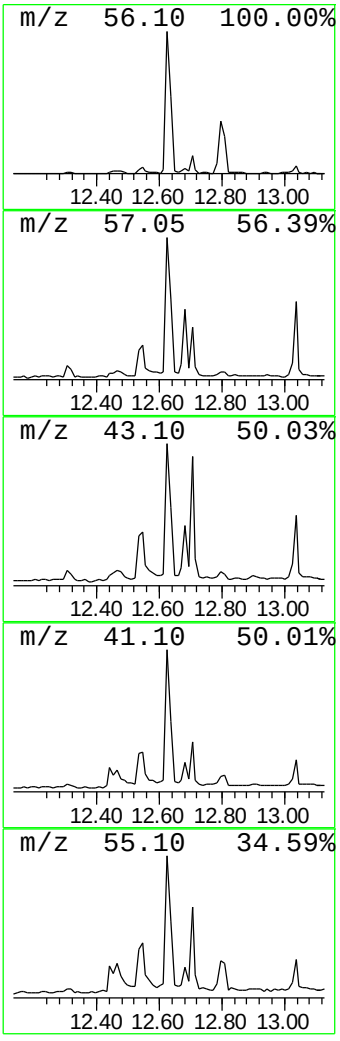
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	9.83 ng	251335	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

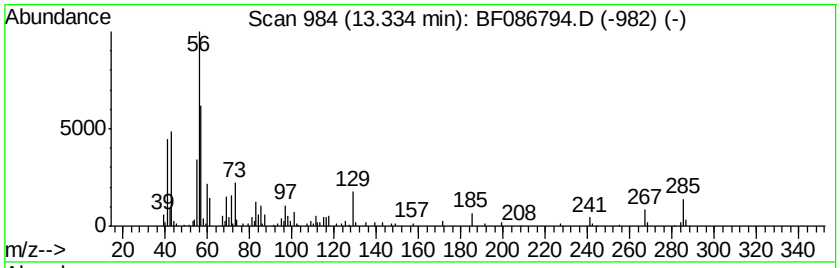
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

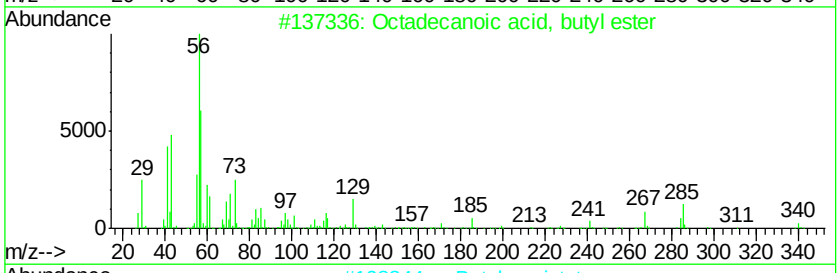
****

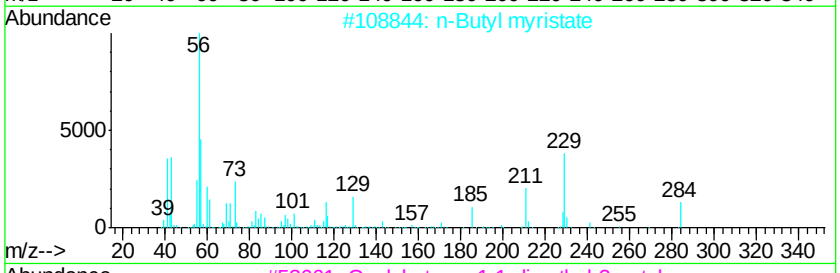
Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 5

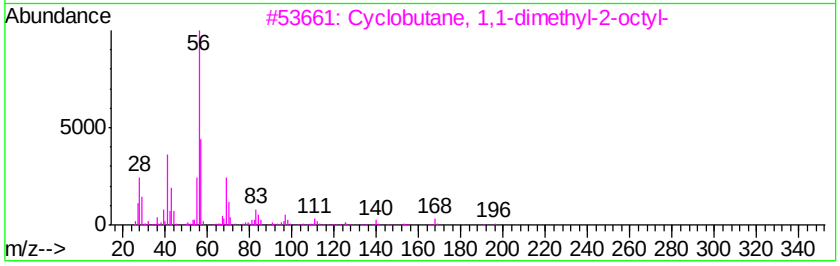
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	7.62 ng	194917	Chrysene-d12	13.85

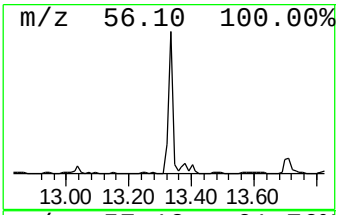
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	78
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38

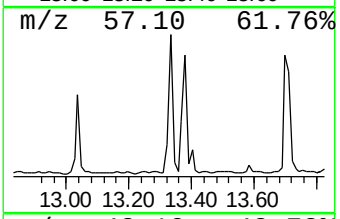


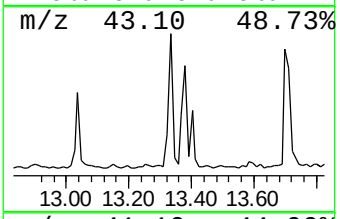


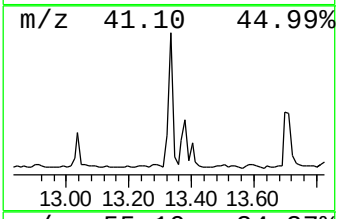


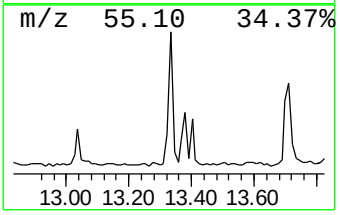












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

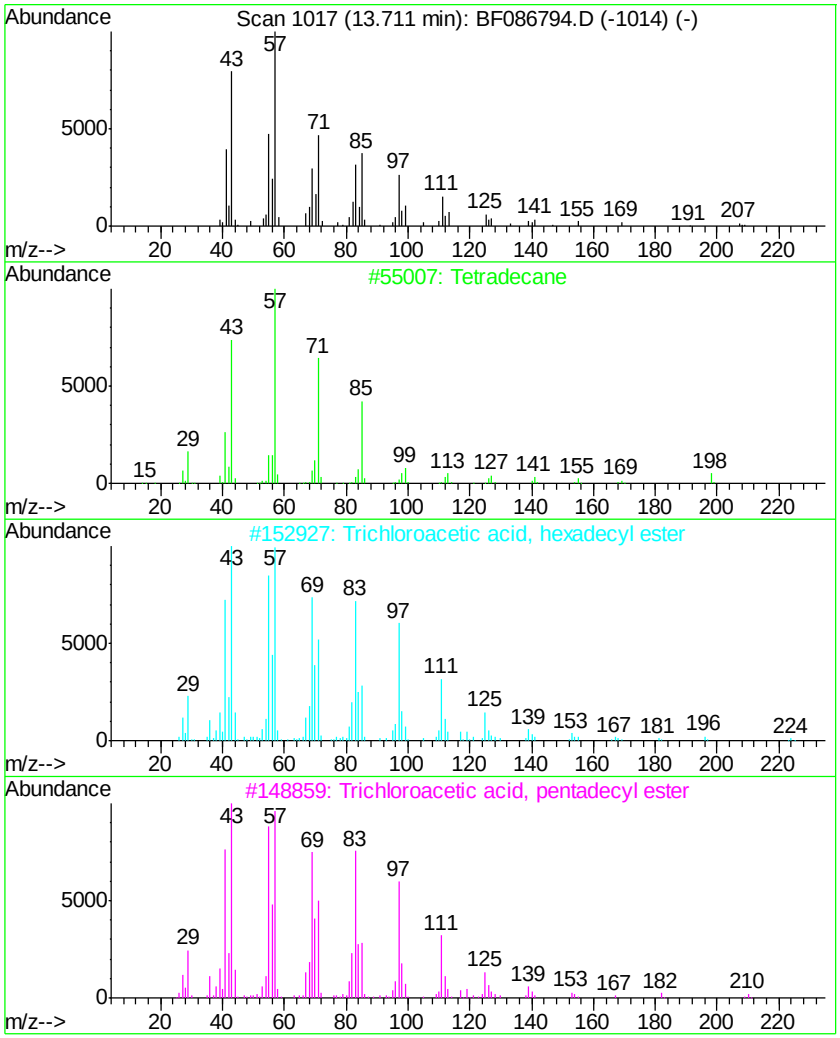
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

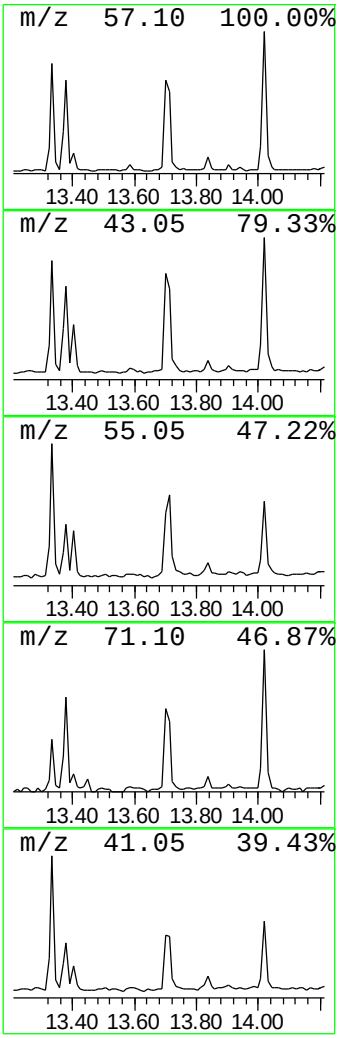
****

Peak Number 9 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.22 ng	159026	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	58
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	53
4	Hexadecane	226	C16H34	000544-76-3	52
5	Pentadecane	212	C15H32	000629-62-9	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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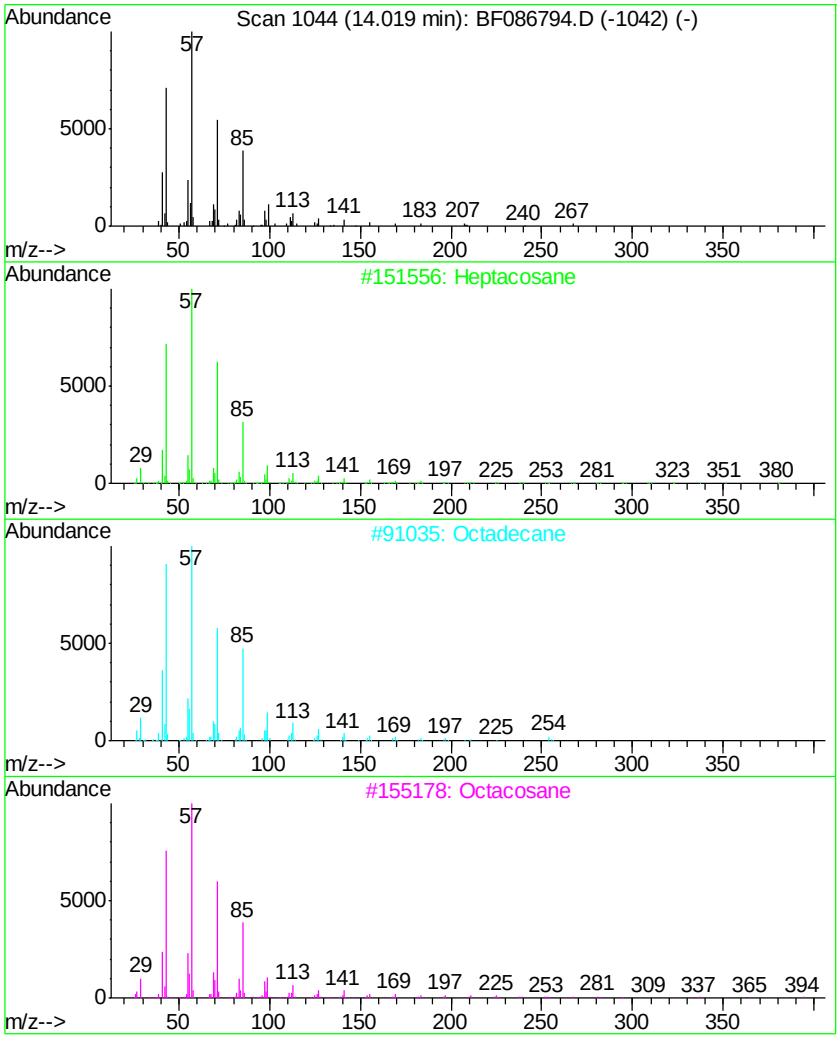
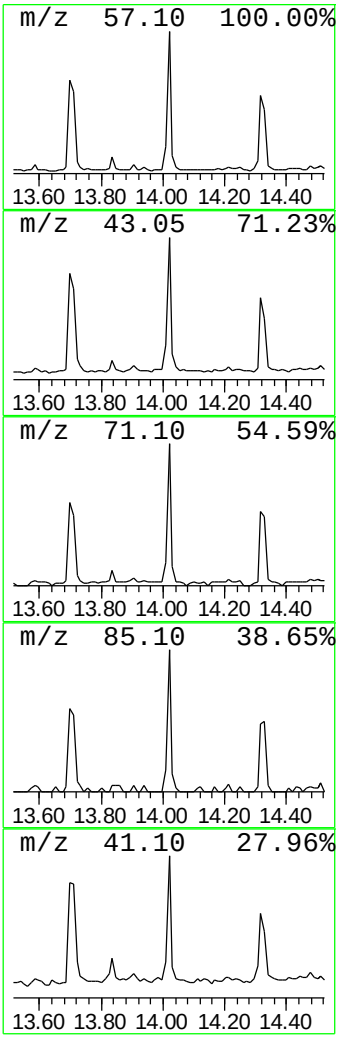
Peak Number 10 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	4.55 ng	116351	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane	240	C17H36	000629-78-7	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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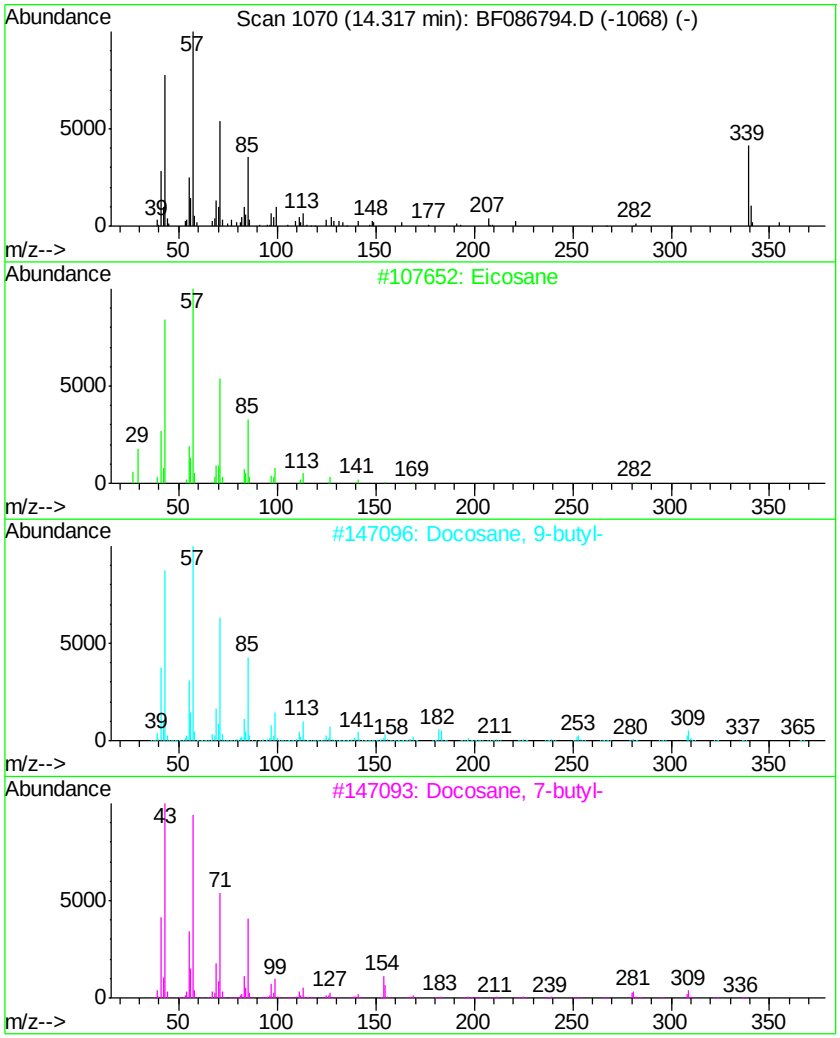
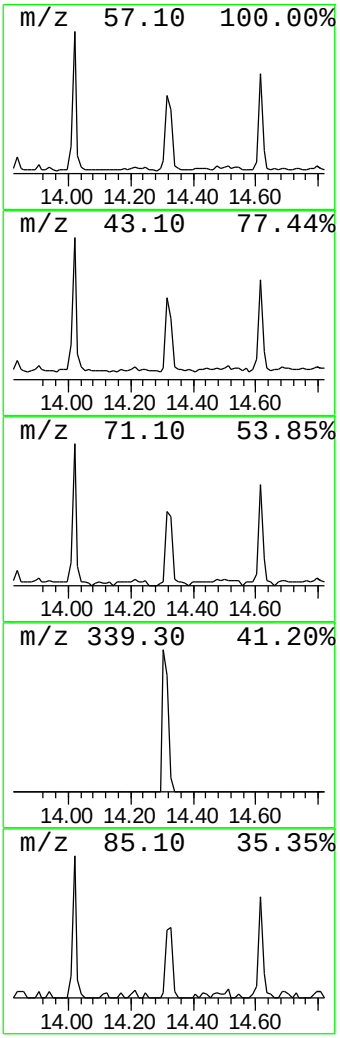
Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	4.93 ng	125961	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	53
3	Docosane, 7-butyl-	366	C26H54	055282-15-0	53
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	53
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
Operator : UM/SJ
Sample : H2882-06
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MWHR2-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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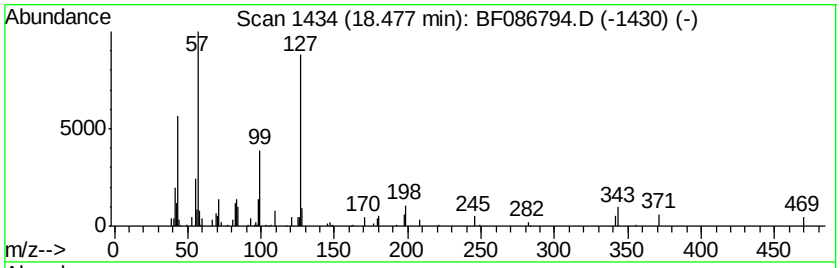
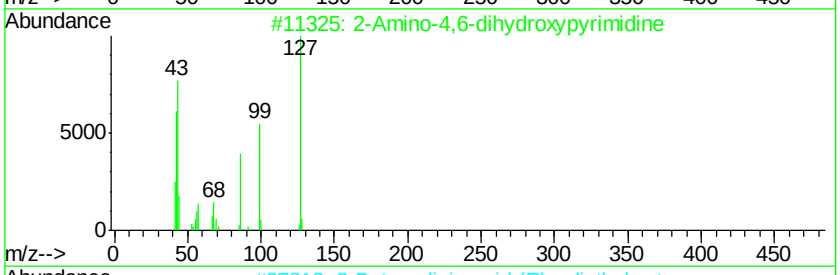
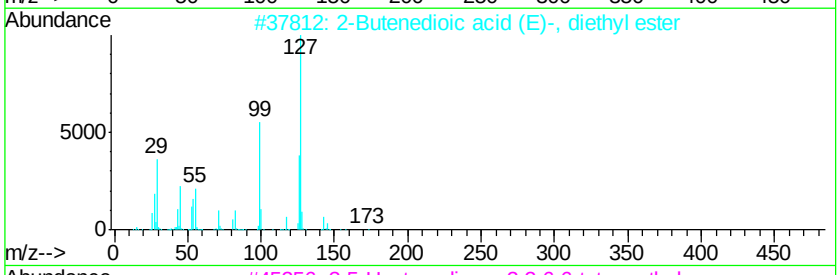
Peak Number 13 2-Amino-4,6-dihydroxypyrimi... Concentration Rank 8

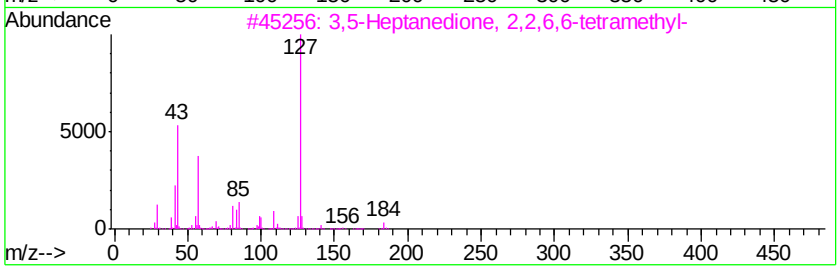
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	6.12 ng	129470	Perylene-d12	15.22

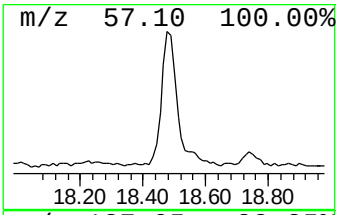
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-4,6-dihydroxypyrimidine	127	C4H5N3O2	000056-09-7	53
2	2-Butenedioic acid (E)-, diethyl...	172	C8H12O4	000623-91-6	42
3	3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	38
4	1,2-Di-n-butyl-3-methyldiaziridine	170	C10H22N2	015656-75-4	38
5	3-Methyl-4-amino-5-methylamino-1...	127	C4H9N5	065901-89-5	38

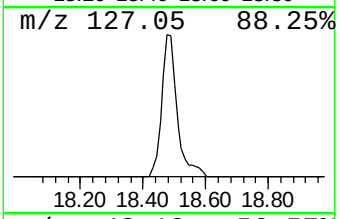


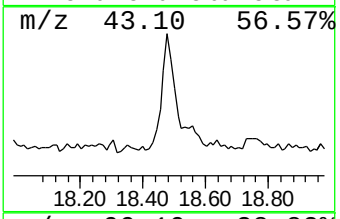


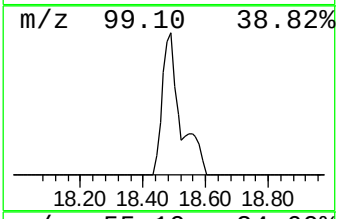


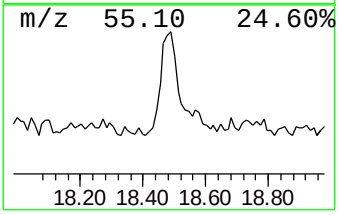












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086794.D
Acq On : 8 May 2016 00:55
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Sample : H2882-06
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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
2-Pentanone, 4-hy...	4.86	7.0	ng	192564	1	6.70	1102410	40.0
unknown6.48	6.48	164.8	ng	4541800	1	6.70	1102410	40.0
1-Nonene	7.93	20.1	ng	712094	2	7.98	1416290	40.0
Hexadecane	10.65	4.4	ng	156741	4	11.22	1425260	40.0
Tetradecanoic acid	12.55	4.5	ng	115874	5	13.85	1022610	40.0
Hexadecanoic acid...	12.63	9.8	ng	251335	5	13.85	1022610	40.0
Octadecanoic acid...	13.33	7.6	ng	194917	5	13.85	1022610	40.0
Tetradecane	13.71	6.2	ng	159026	5	13.85	1022610	40.0
Heptacosane	14.02	4.5	ng	116351	5	13.85	1022610	40.0
Eicosane	14.32	4.9	ng	125961	5	13.85	1022610	40.0
2-Amino-4,6-dihyd...	18.48	6.1	ng	129470	6	15.22	846283	40.0