LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

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-BF042716.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	2.224	10	12	32	rVB	54159	223164	5.73%	0.622%
2	4.967	250	252	260	rVB	64613	115826	2.98%	0.323%
3	5.390	286	289	291	rBV	3304439	3893212	100.00%	10.857%
4	6.430	377	380	382	rBV	3428230	3748090	96.27%	10.452%
5	6.556	388	391	394	rBV	3848395	3663238	94.09%	10.215%
6	6.624	395	397	399	rVB	97624	87570	2.25%	0.244%
7	6.784	409	411	414	rBV	1026850	990113	25.43%	2.761%
8	6.944	422	425	427	rBV	3258344	2963626	76.12%	8.264%
9	7.356	458	461	463	rBV	2441669	2568641	65.98%	7.163%
10	7.459	467	470	477	rVB	70531	150981	3.88%	0.421%
11	8.076	521	524	526	rBV	1332637	1267652	32.56%	3.535%
12	9.150	616	618	621	rBV	3260620	3489301	89.63%	9.730%
13	9.276	627	629	630	rVB	82955	74119	1.90%	0.207%
14	9.550	650	653	655	rBV	684098	617858	15.87%	1.723%
15	9.768	671	672	674	rVB	57832	41555	1.07%	0.116%
16	9.825	675	677	680	rVV	1299212	1216491	31.25%	3.392%
17	10.236	711	713	714	rBV	51080	59314	1.52%	0.165%
18	10.270	714	716	717	rVB	73779	88247	2.27%	0.246%
19	10.488	732	735	736	rBV2	47930	89880	2.31%	0.251%
20	10.613	743	746	749	rBV	1989394	1972077	50.65%	5.499%
21	10.670	749	751	753	rVV	58761	115178	2.96%	0.321%
22	10.739	755	757	763	rVB	160429	218634	5.62%	0.610%
23	10.933	772	774	776	rBV	24381	39073	1.00%	0.109%
24	11.185	794	796	797	rBV	107321	84076	2.16%	0.234%
25	11.219	797	799	802	rVB	31275	44497	1.14%	0.124%
26	11.311	805	807	809	rBV	872237	976374	25.08%	2.723%
27	11.368	810	812	816	rVB2	34914	53784	1.38%	0.150%
28	11.539	825	827	831	rBV	506508	490294	12.59%	1.367%
29	11.608	831	833	840	rVB	69784	86184	2.21%	0.240%
30	11.848	852	854	858	rBV2	217080	346348	8.90%	0.966%
31	12.362	896	899	902	rBV	643954	812078	20.86%	2.265%
32	12.408	902	903	907	rVV2	58255	69011	1.77%	0.192%
33	12.556	914	916	920	rBV	24800	46879	1.20%	0.131%
34	12.728	928	931	933	rBV2	52595	114684	2.95%	0.320%

LSC Area Percent Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.774	933	935	936	rVV	88531	77838	2.00%	0.217%
36	12.888	943	945	948	rBV	1570391	2143192	55.05%	5.977%
37	13.128	965	966	968	rVB	78386	74772	1.92%	0.209%
38	13.345	983	985	986	rBV	58122	59199	1.52%	0.165%
39	13.425	990	992	994	rBV2	47587	63887	1.64%	0.178%
40	13.471	994	996	1001	rVV	70549	107450	2.76%	0.300%
41	13.791	1022	1024	1030	rBV	132830	256394	6.59%	0.715%
42	13.939	1034	1037	1043	rBV	765331	1025812	26.35%	2.861%
43	14.419	1077	1079	1081	rBV	76254	105561	2.71%	0.294%
44	14.694	1101	1103	1109	rVB2	324936	405297	10.41%	1.130%
45	15.345	1157	1160	1162	rBV	514227	722754	18.56%	2.015%

Sum of corrected areas: 35860205

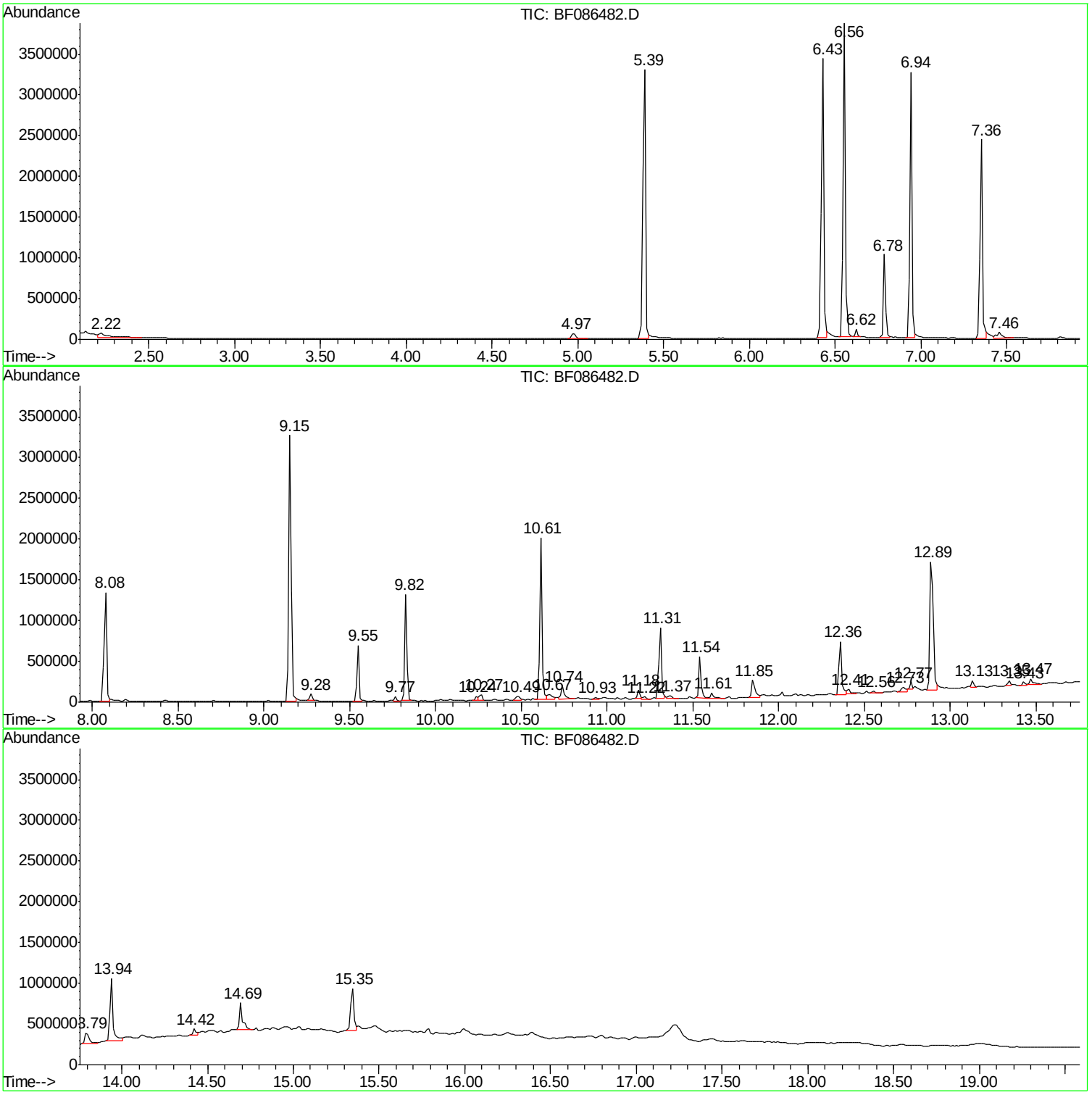
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

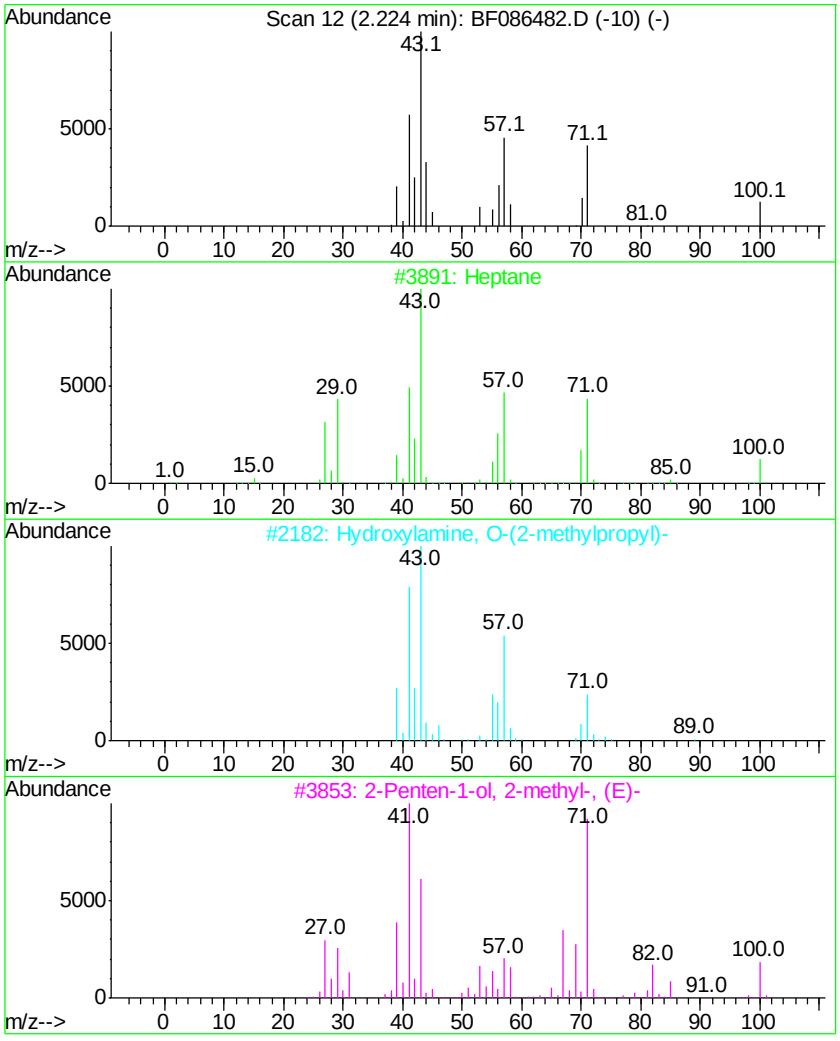
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

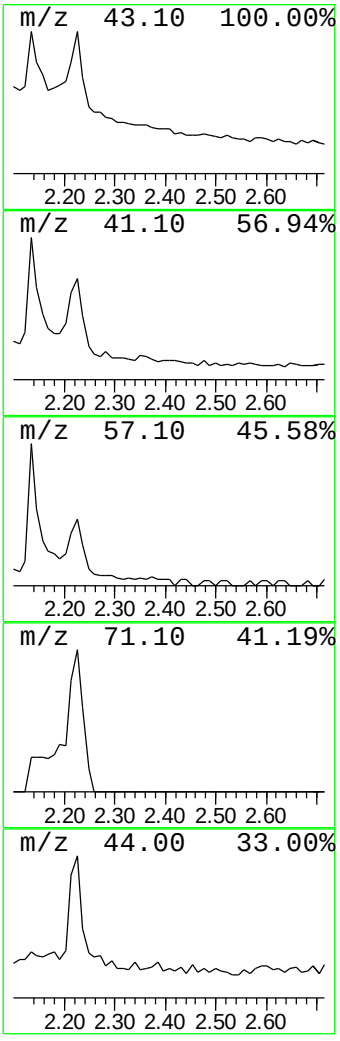
****

Peak Number 1 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	4.51 ng	223164	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	74
2	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	53
3	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	35
4	2-Penten-1-ol, 2-methyl-	100	C6H12O	001610-29-3	35
5	Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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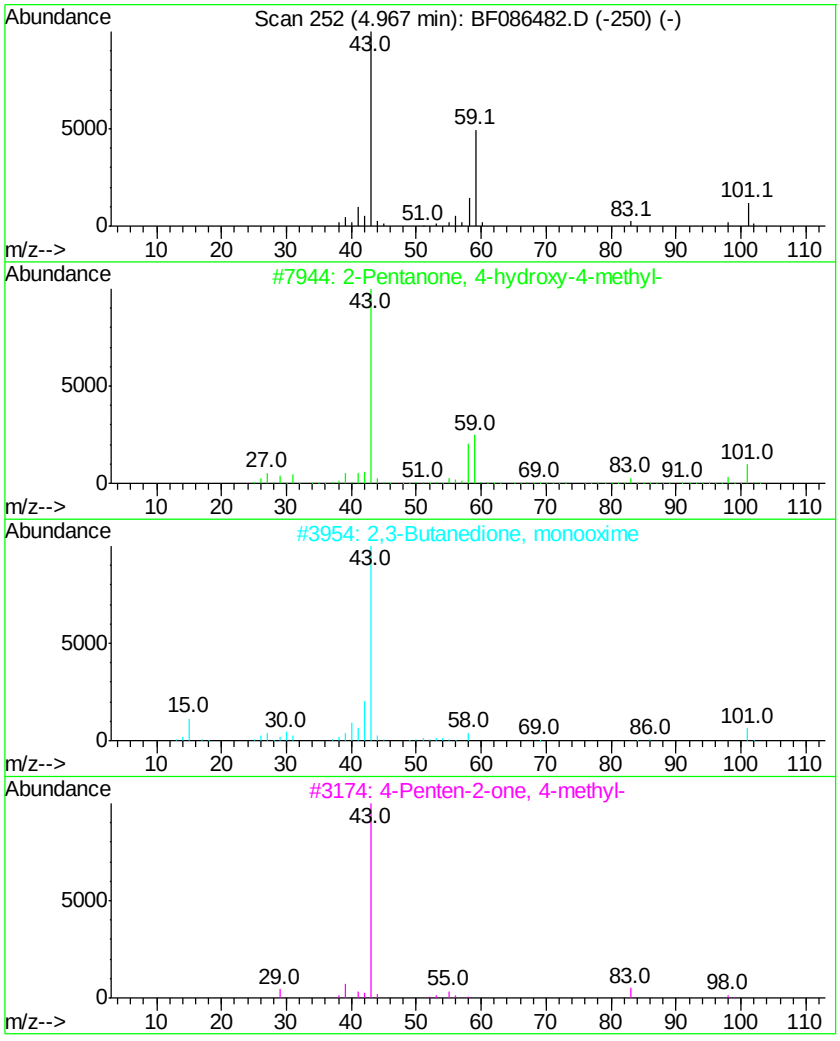
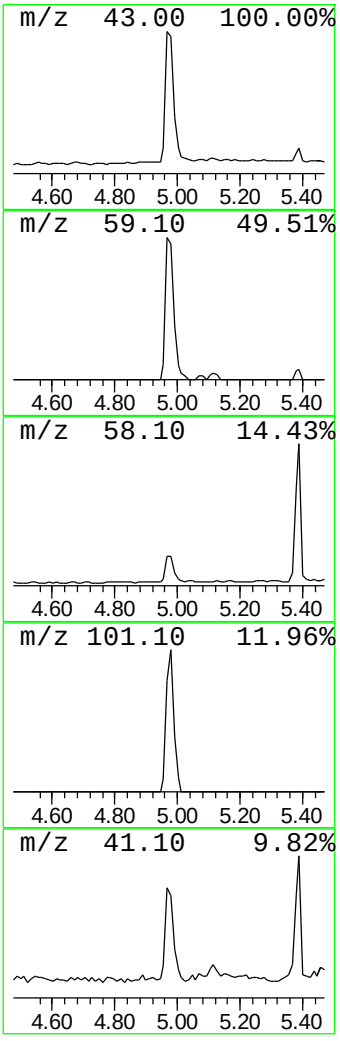
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.34 ng	115826	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Methyl acetoxyacetate	132	C5H8O4	005837-80-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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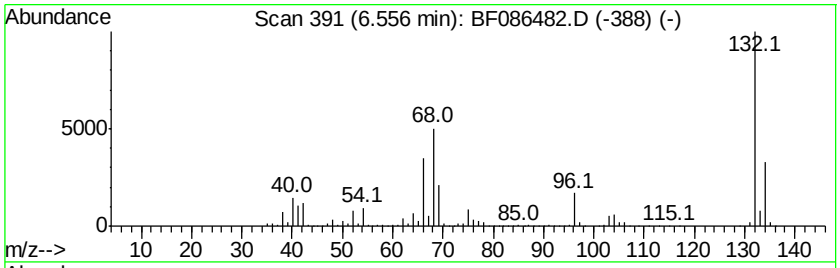
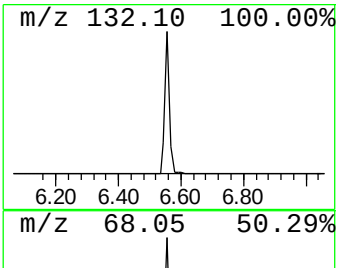
Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	74.00 ng	3663240	1,4-Dichlorobenzene-d4	6.78

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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
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Operator : UM/SJ
Sample : H2654-11
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Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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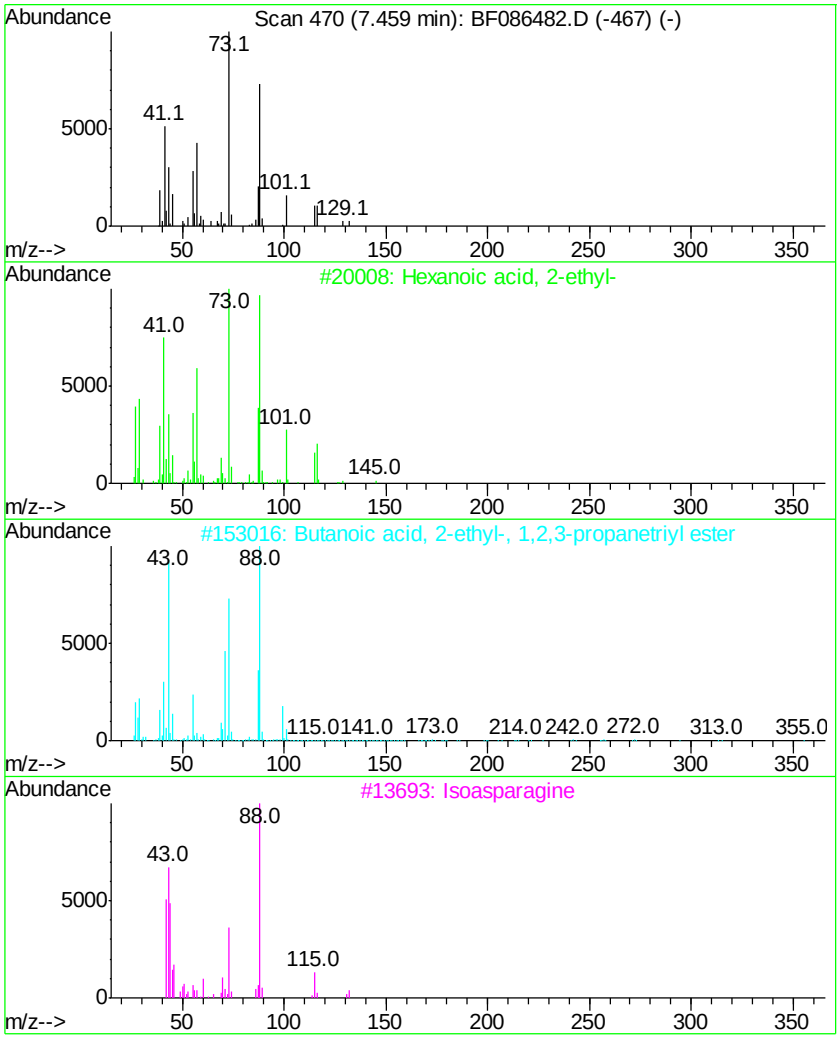
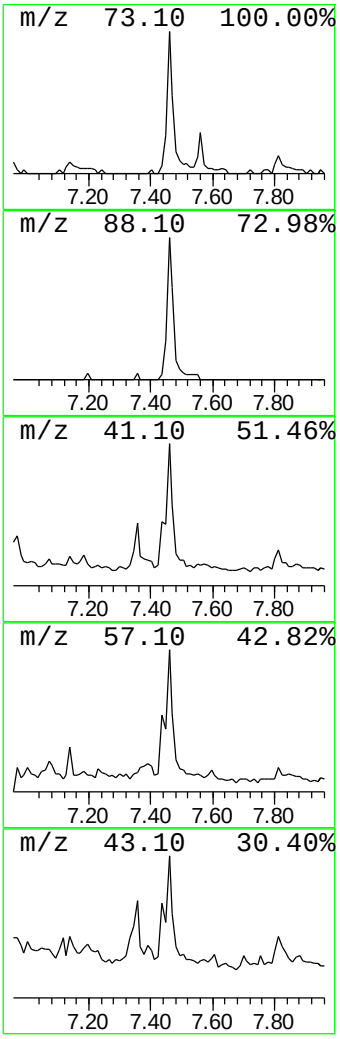
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.38 ng	150981	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	47
3	Isoasparagine	132	C4H8N2O3	1000130-17-5	33
4	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	33
5	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	32





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Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
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TIC Library : C:\DATABASE\NIST02.L
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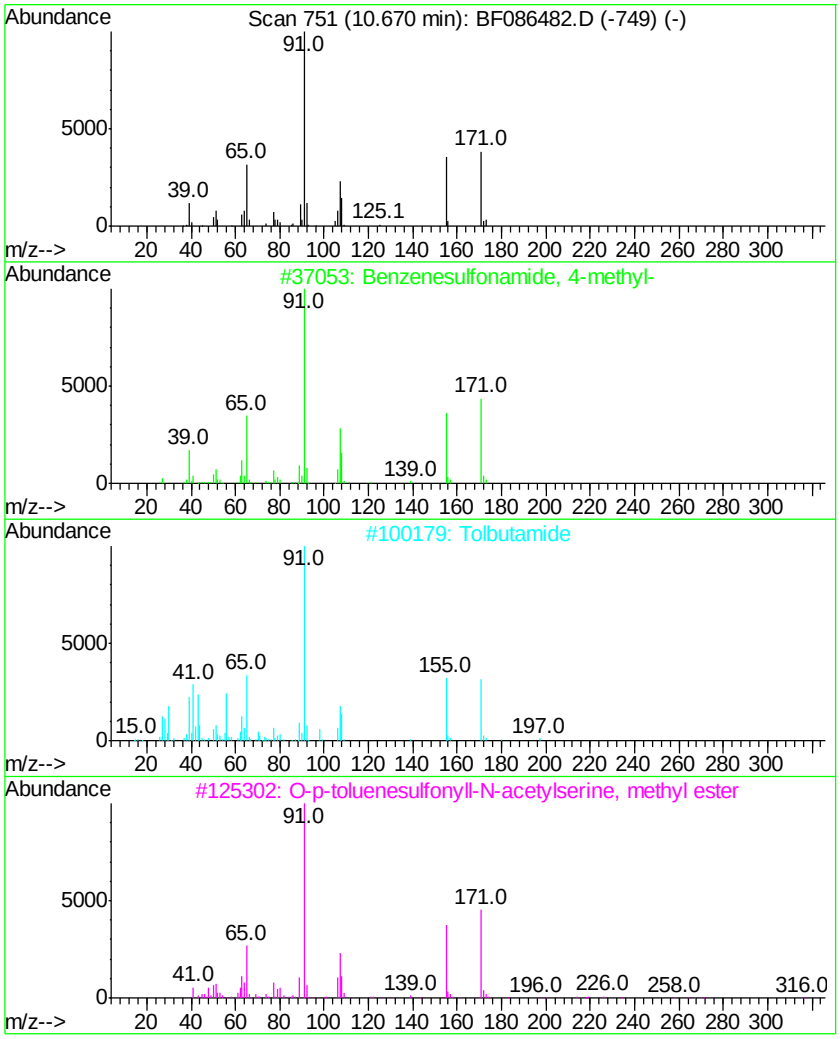
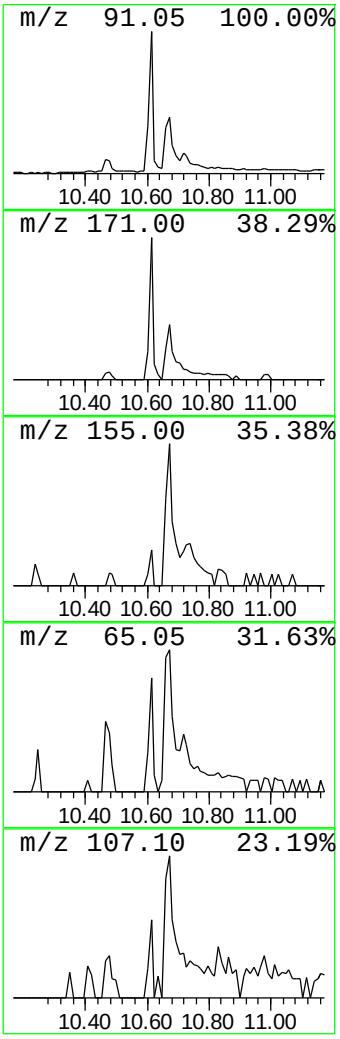
****

Peak Number 6 Benzenesulfonamide, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.36 ng	115178	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	94
2	Tolbutamide	270	C12H18N2O3S	000064-77-7	90
3	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	83
4	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	56
5	Thiophene-3-ol, 2,3-dihydro-, 4-...	288	C11H12O5S2	039582-96-2	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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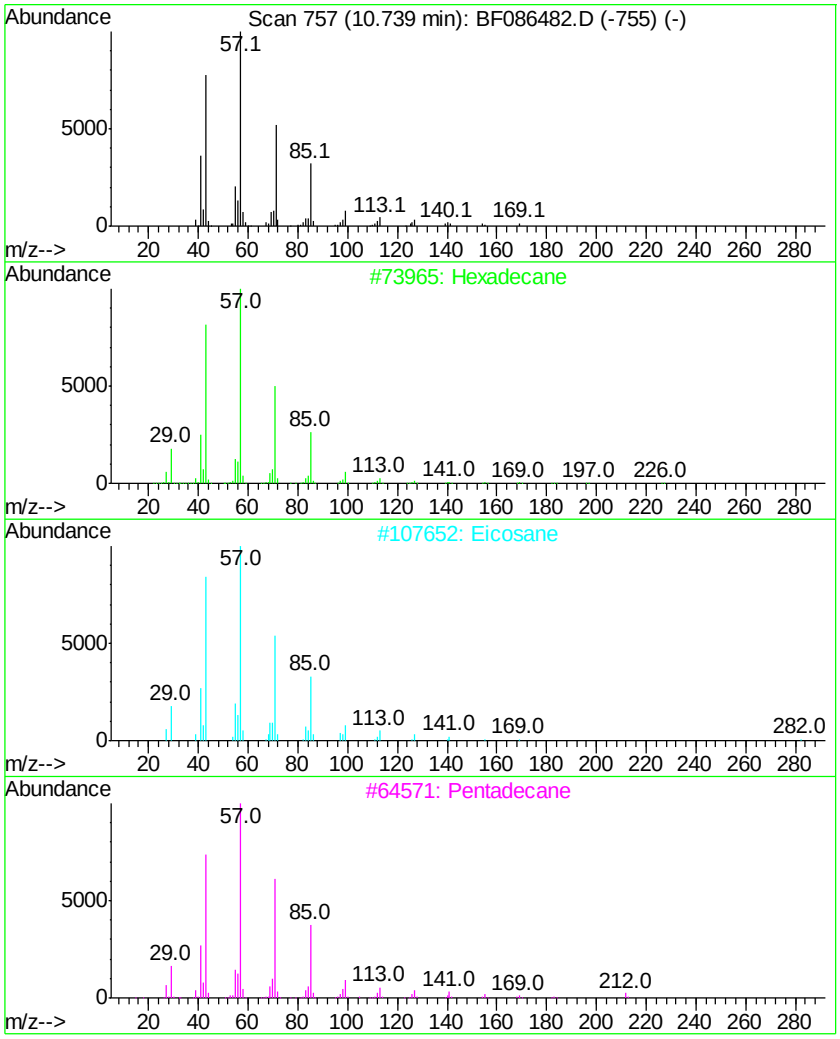
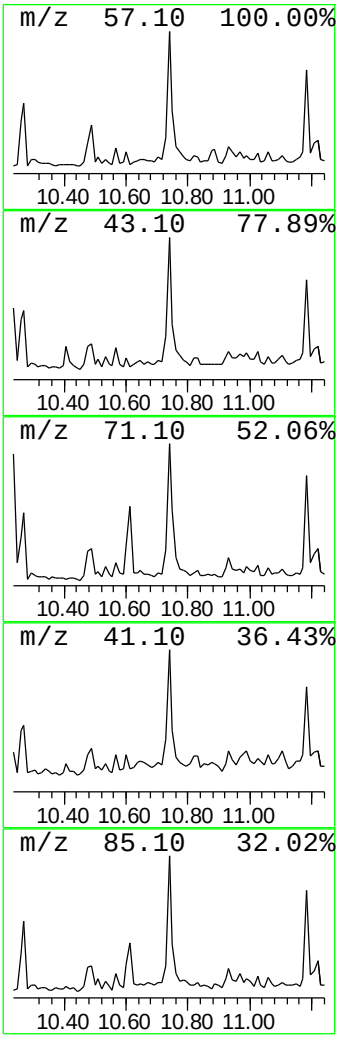
Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.48 ng	218634	Phenanthrene-d10	11.31

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	83
5	Heptacosane	380	C27H56	000593-49-7	83





Library Search Compound Report

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Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
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Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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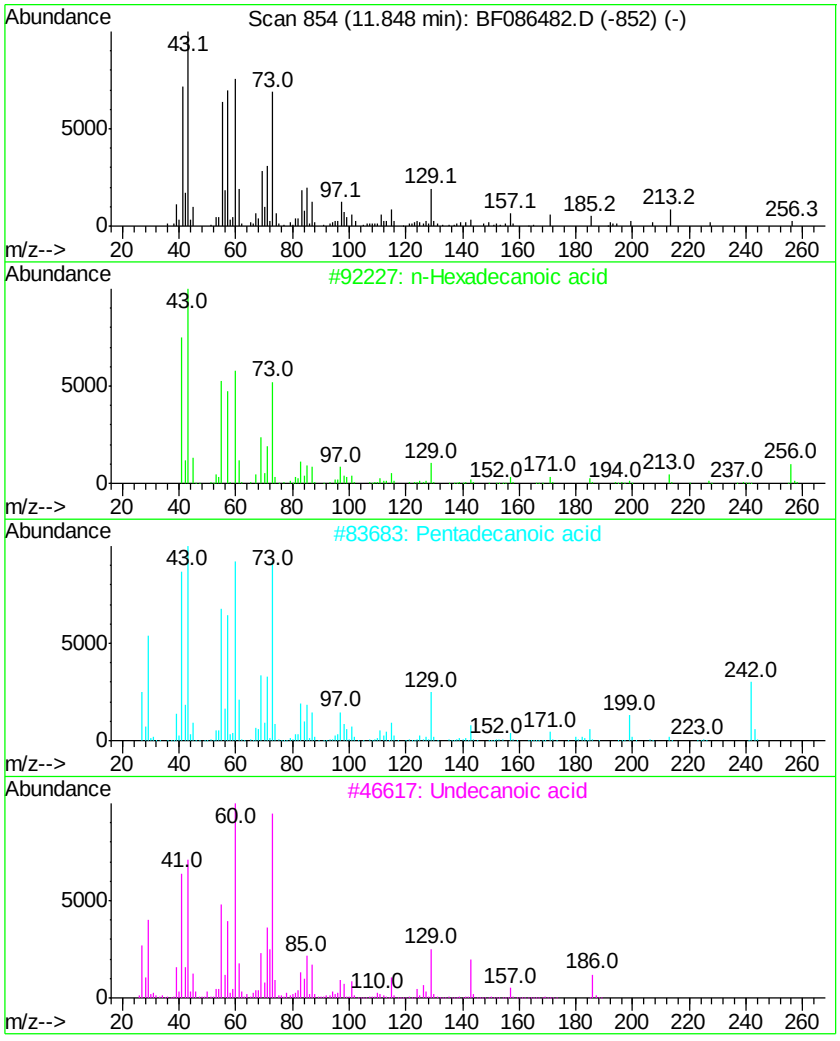
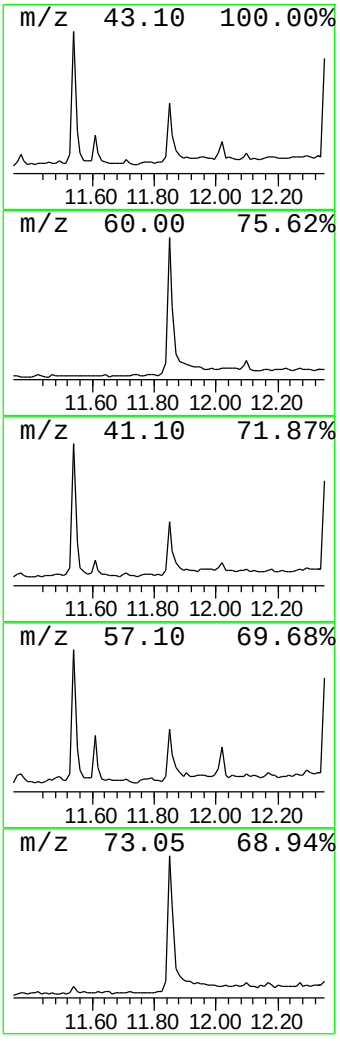
Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	7.09 ng	346348	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

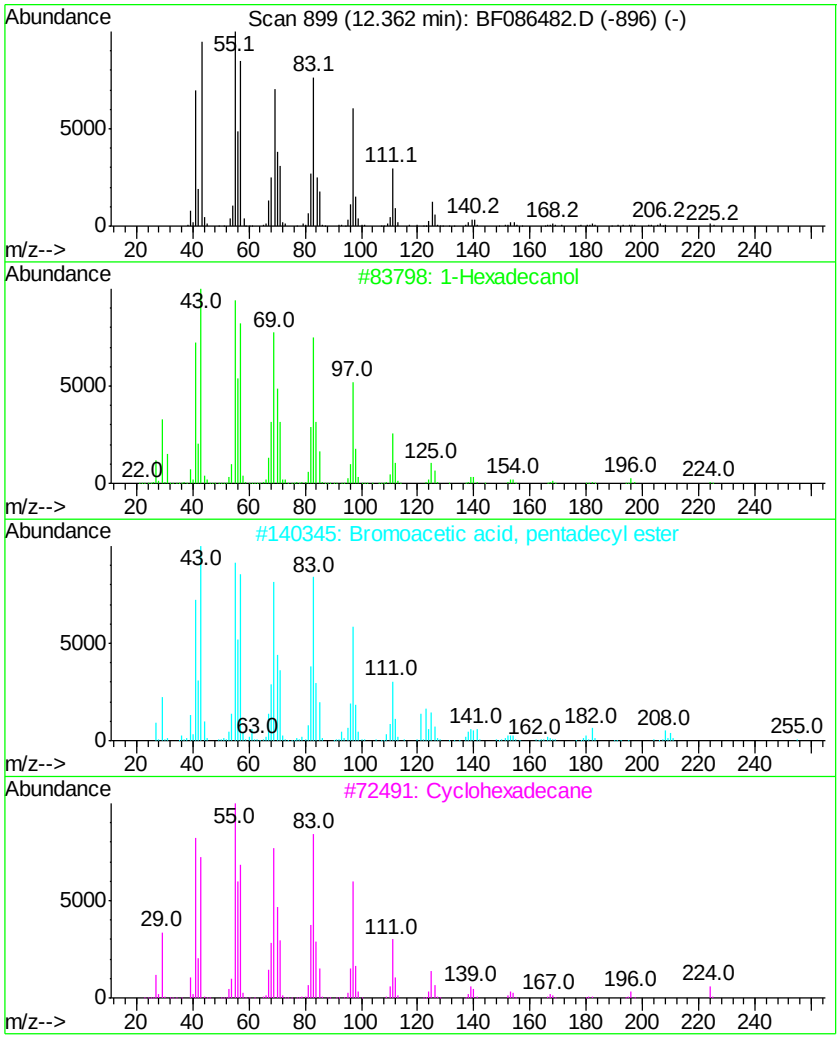
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

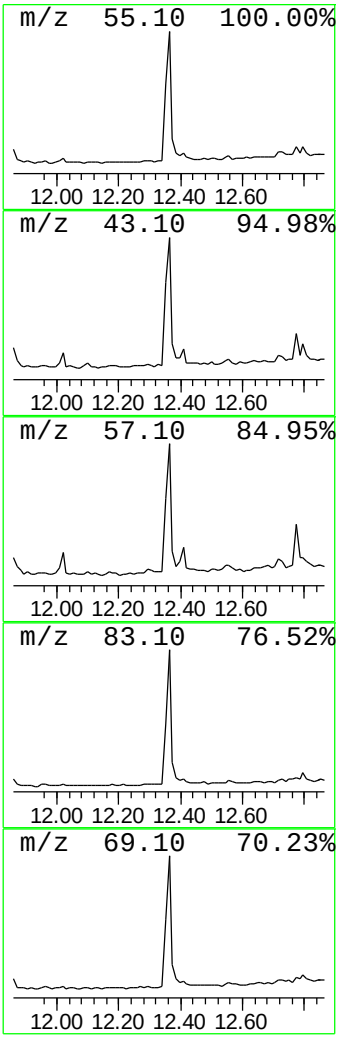
****

Peak Number 10 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	16.63 ng	812078	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
3	Cyclohexadecane	224	C16H32	000295-65-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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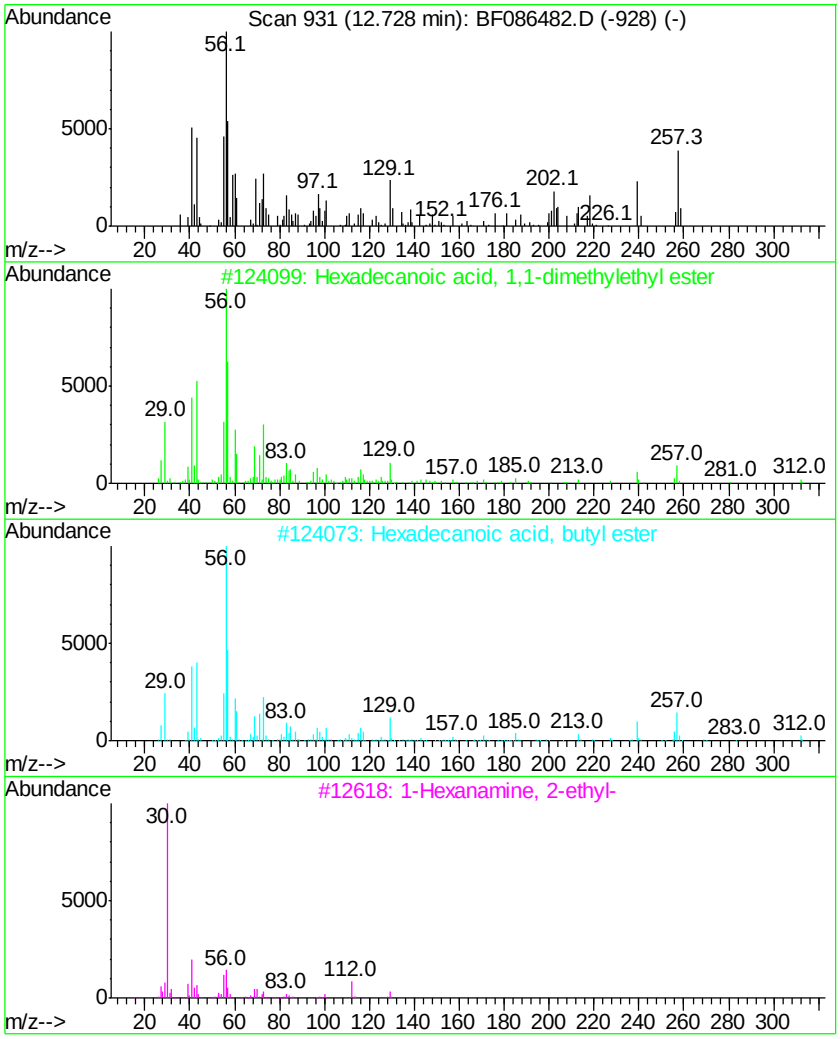
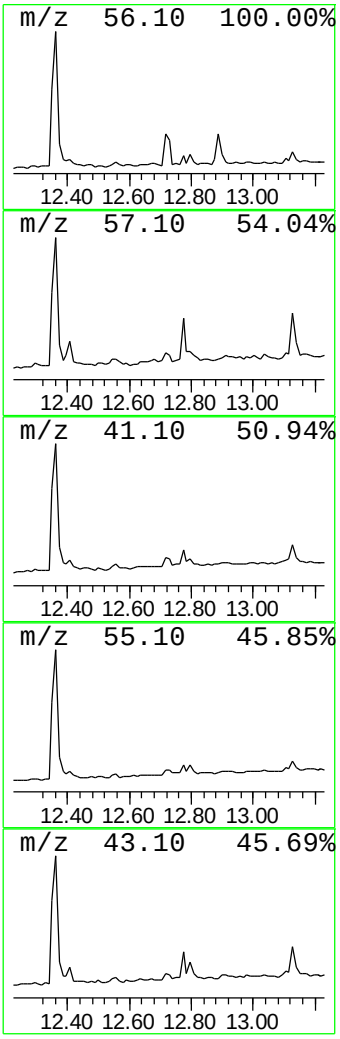
Peak Number 11 unknown12.73 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.24 ng	114684	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	46
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	35
3	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	35
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	14





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Data File : BF086482.D
Acq On : 29 Apr 2016 00:17
Operator : UM/SJ
Sample : H2654-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
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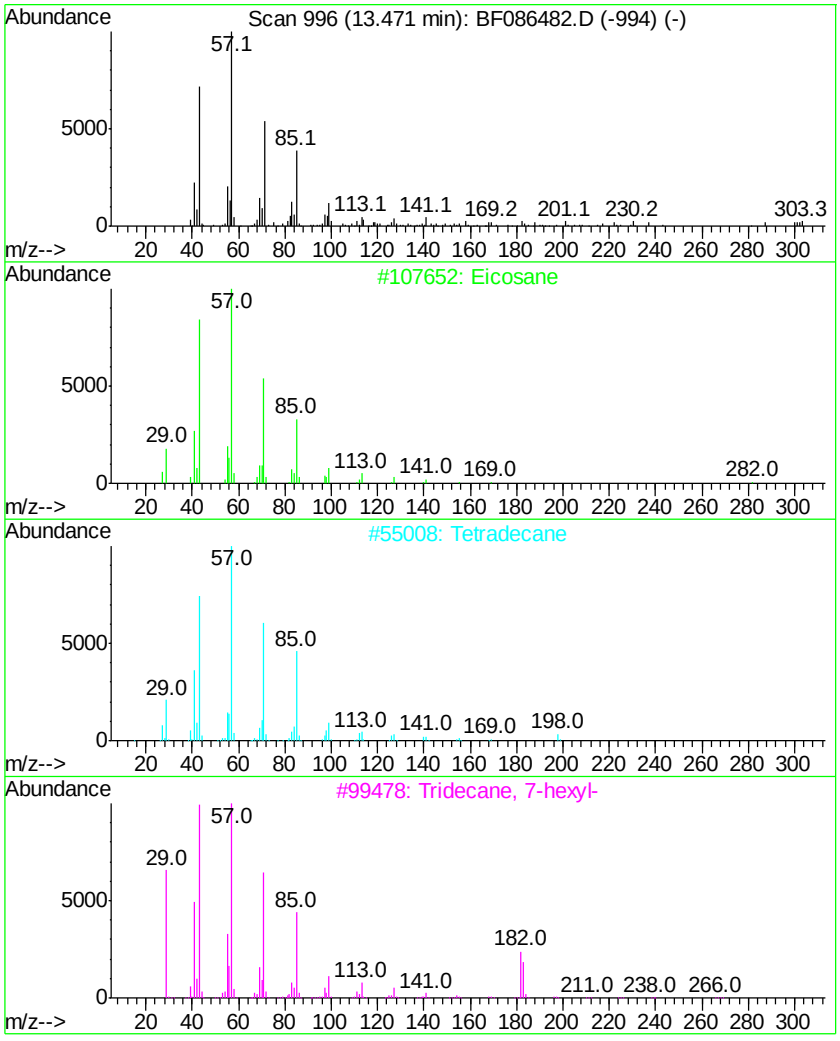
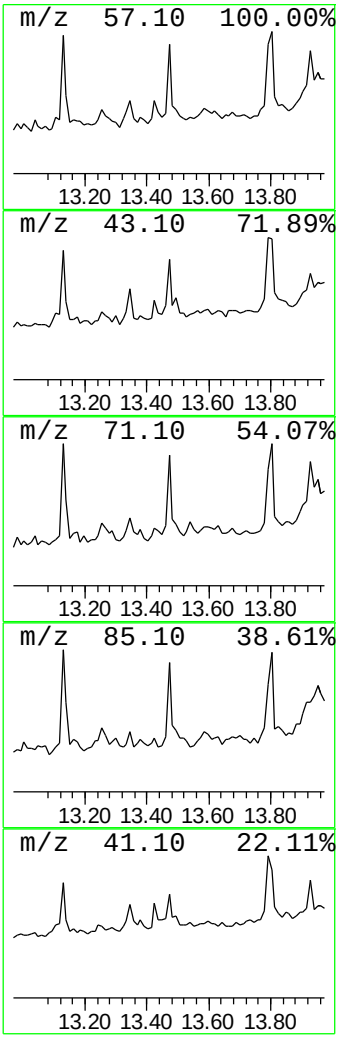
Peak Number 12 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.09 ng	107450	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Tetradecane	198	C14H30	000629-59-4	80
3	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Pentadecane	212	C15H32	000629-62-9	80





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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId : 26WARD-2A-CS-16(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
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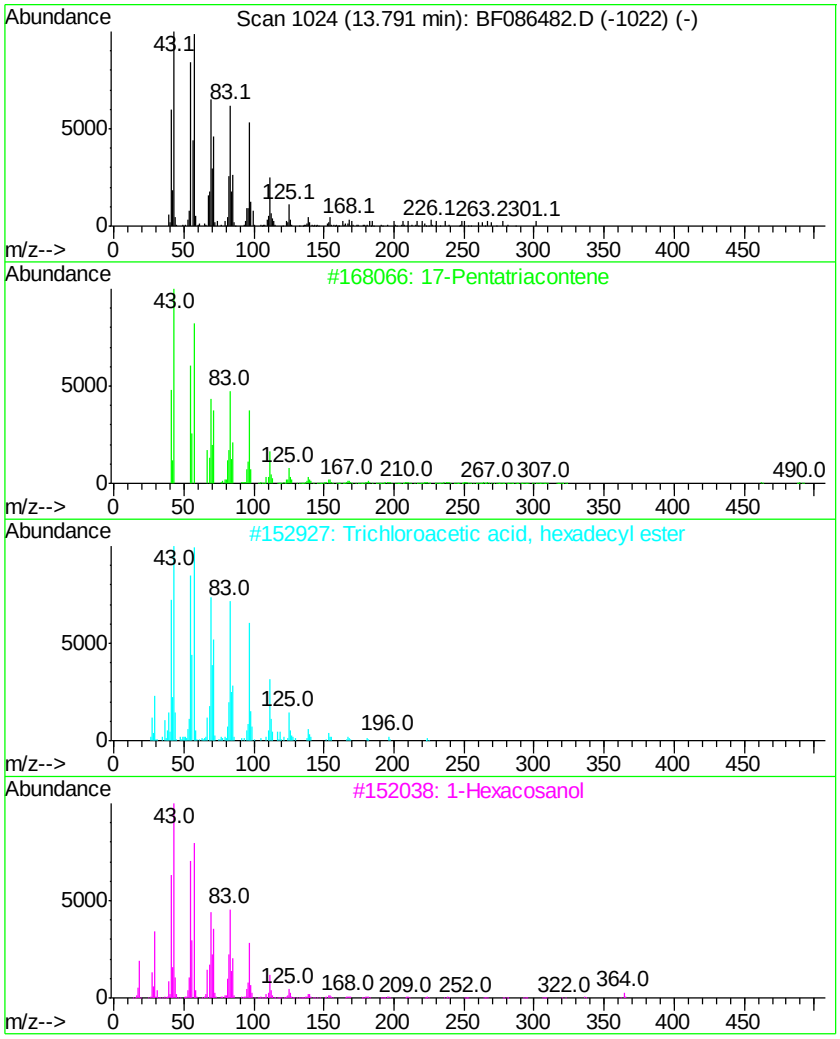
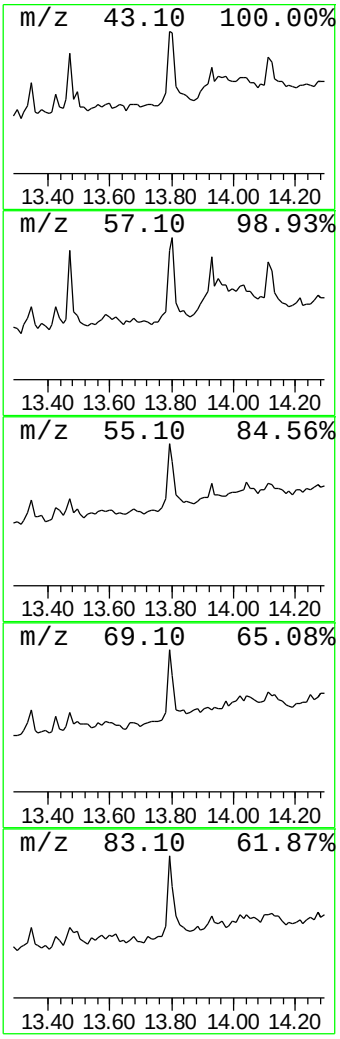
Peak Number 13 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	5.00 ng	256394	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
5	1-Tetracosanol	354	C24H50O	000506-51-4	87





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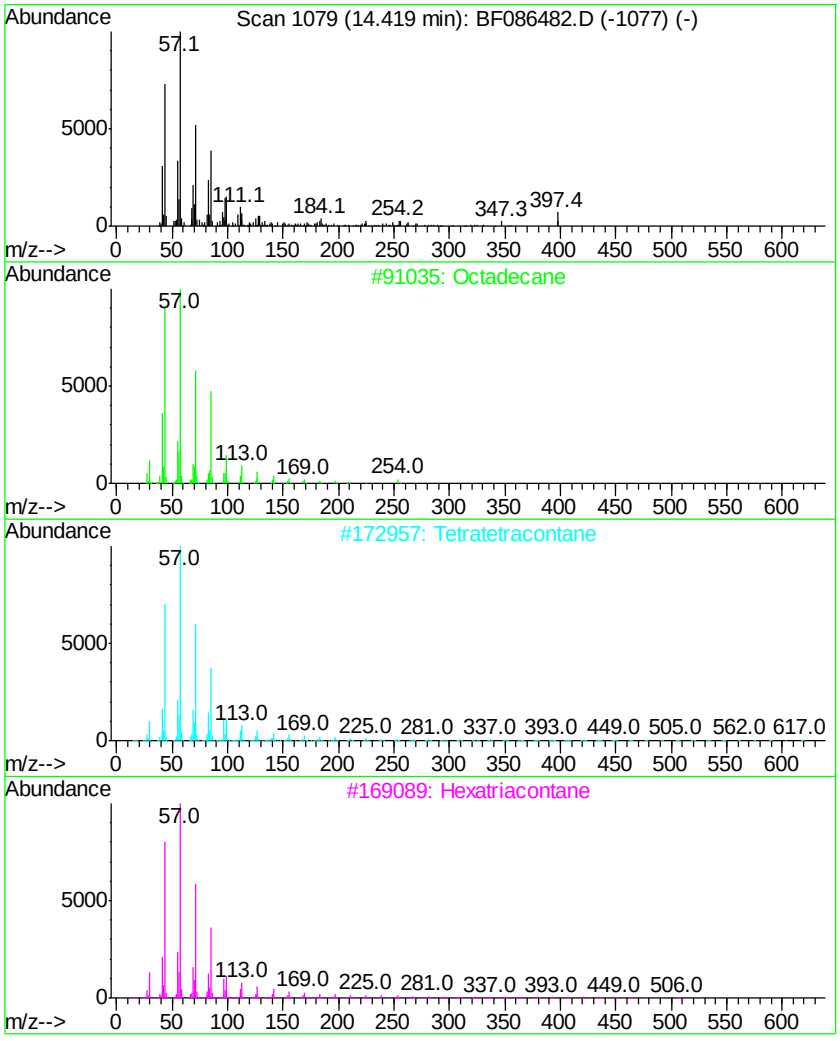
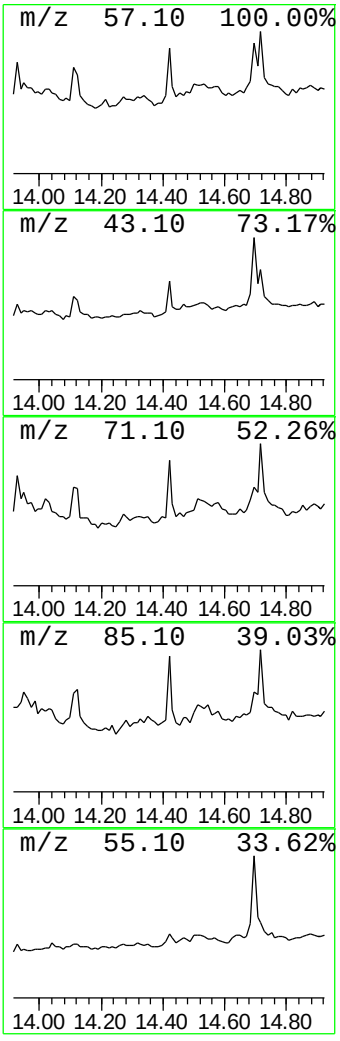
Peak Number 14 Octadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.06 ng	105561	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Tetratetracontane	619	C44H90	007098-22-8	80
3	Hexatriacontane	507	C36H74	000630-06-8	72
4	Heptacosane	380	C27H56	000593-49-7	72
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	72





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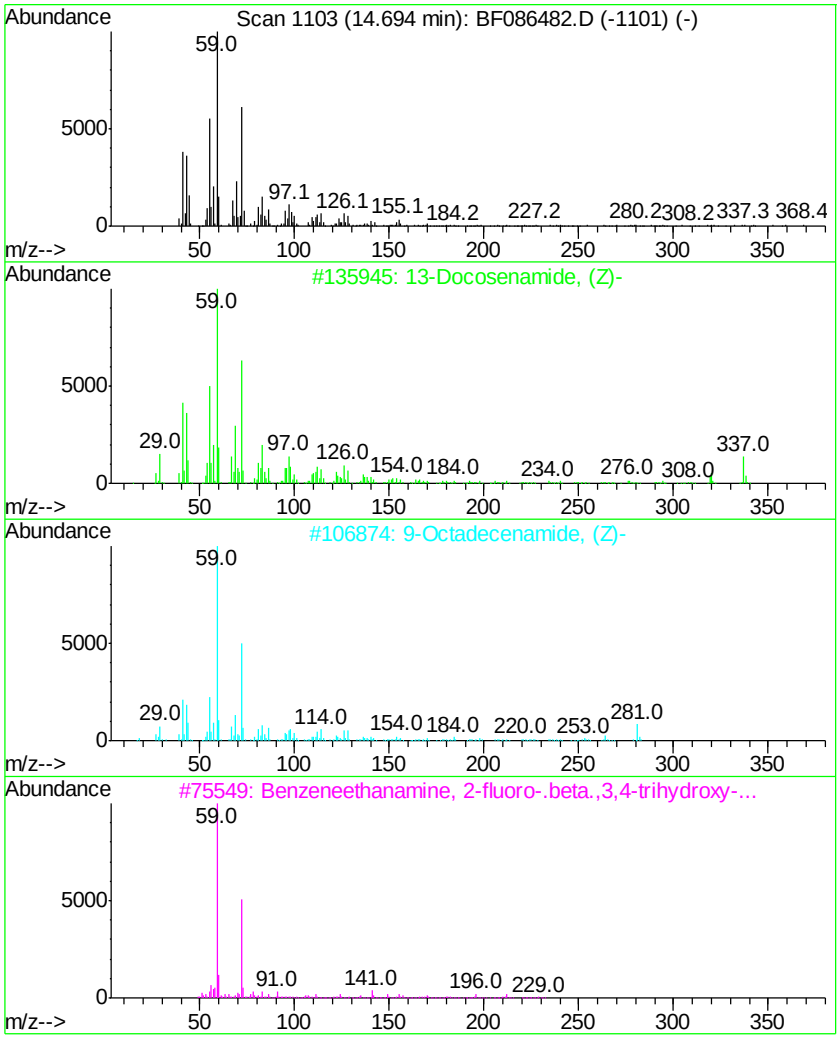
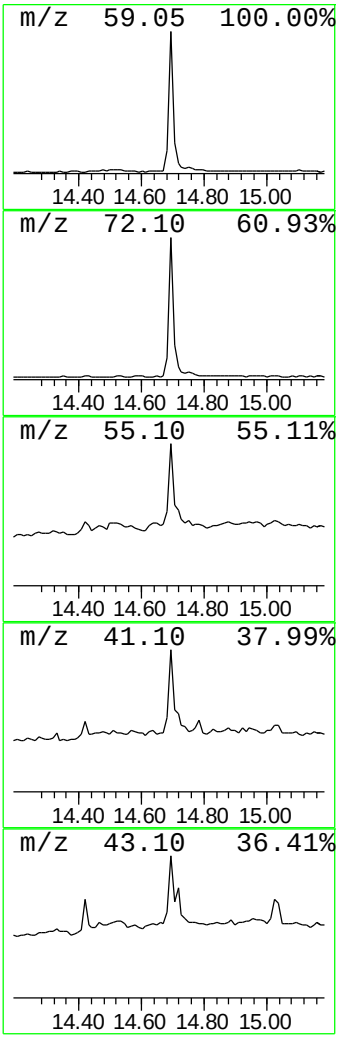
Peak Number 15 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	11.22 ng	405297	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
4	Octadecanamide	283	C18H37NO	000124-26-5	59
5	Octanamide	143	C8H17NO	000629-01-6	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Heptane	2.22	4.5	ng	223164	1	6.78	990113	20.0
2-Pentanone, 4-hy...	4.97	2.3	ng	115826	1	6.78	990113	20.0
unknown6.56	6.56	74.0	ng	3663240	1	6.78	990113	20.0
Hexanoic acid, 2-...	7.46	2.4	ng	150981	2	8.08	1267650	20.0
Benzenesulfonamid...	10.67	2.4	ng	115178	4	11.31	976374	20.0
Hexadecane	10.74	4.5	ng	218634	4	11.31	976374	20.0
n-Hexadecanoic acid	11.85	7.1	ng	346348	4	11.31	976374	20.0
1-Hexadecanol	12.36	16.6	ng	812078	4	11.31	976374	20.0
unknown12.73	12.73	2.2	ng	114684	5	13.94	1025810	20.0
Eicosane	13.47	2.1	ng	107450	5	13.94	1025810	20.0
17-Pentatriacontene	13.79	5.0	ng	256394	5	13.94	1025810	20.0
Octadecane	14.42	2.1	ng	105561	5	13.94	1025810	20.0
13-Docosenamide, ...	14.69	11.2	ng	405297	6	15.35	722754	20.0