LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

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-BF101015.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	3.291	98	101	113	rVB	56895	111506	2.56%	0.504%
2	4.343	188	193	195	rBV	2322101	4222941	96.99%	19.098%
3	5.029	247	253	255	rBV	1840854	4353860	100.00%	19.690%
4	6.457	375	378	380	rBV	332444	365603	8.40%	1.653%
5	6.583	388	389	392	rBV	47147	52153	1.20%	0.236%
6	6.823	407	410	412	rBV	484986	436150	10.02%	1.972%
7	6.972	421	423	426	rBV	997300	1375343	31.59%	6.220%
8	7.155	437	439	447	rVB	39575	49164	1.13%	0.222%
9	7.395	457	460	462	rBV	1110176	1093382	25.11%	4.945%
10	8.115	520	523	525	rBV	556645	593035	13.62%	2.682%
11	9.189	615	617	620	rBV	1858199	2136043	49.06%	9.660%
12	9.589	650	652	654	rBV	403521	346979	7.97%	1.569%
13	9.875	674	677	679	rBV	624107	720596	16.55%	3.259%
14	10.298	710	714	716	rBV	49508	57069	1.31%	0.258%
15	10.778	754	756	760	rVB	115733	160155	3.68%	0.724%
16	11.223	791	795	796	rBV	61113	58124	1.33%	0.263%
17	11.361	805	807	809	rBV	794170	742128	17.05%	3.356%
18	11.521	820	821	823	rBV	48705	51973	1.19%	0.235%
19	11.578	823	826	830	rVV2	31484	56388	1.30%	0.255%
20	11.646	830	832	836	rVV2	39807	49914	1.15%	0.226%
21	12.504	905	907	910	rVV	60166	82309	1.89%	0.372%
22	12.972	945	948	950	rBV	2409620	2440379	56.05%	11.036%
23	13.932	1030	1032	1037	rVB	312368	393248	9.03%	1.778%
24	14.104	1045	1047	1053	rBV	475770	599761	13.78%	2.712%
25	15.007	1124	1126	1130	rBV2	272545	347978	7.99%	1.574%
26	15.395	1158	1160	1161	rBV	86224	122859	2.82%	0.556%
27	15.715	1185	1188	1191	rVB	345613	421081	9.67%	1.904%
28	16.401	1246	1248	1257	rVB5	98178	335543	7.71%	1.517%
29	16.824	1283	1285	1295	rVB4	75807	227731	5.23%	1.030%
30	16.984	1297	1299	1305	rVB	50178	108842	2.50%	0.492%

Sum of corrected areas: 22112237

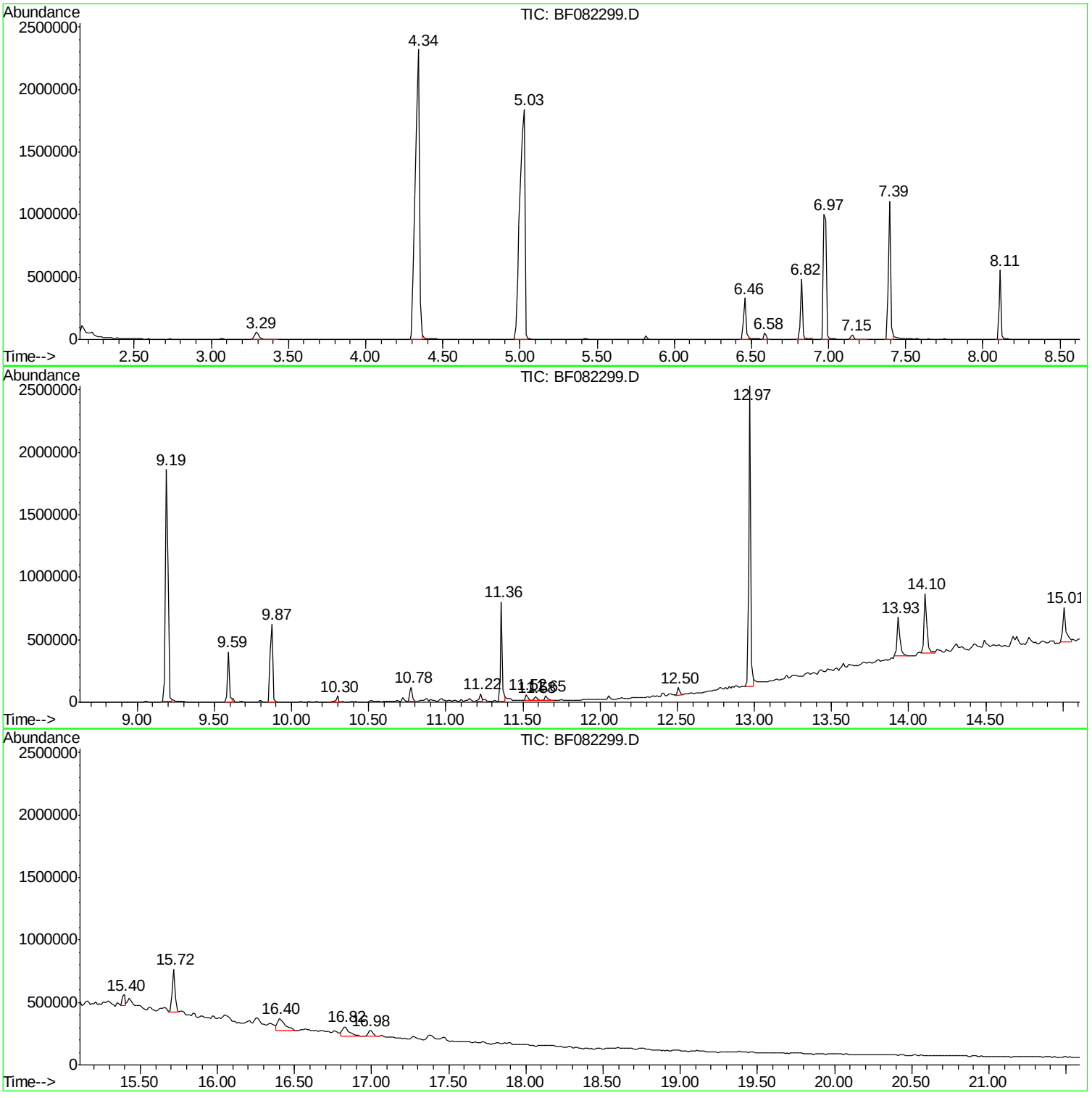
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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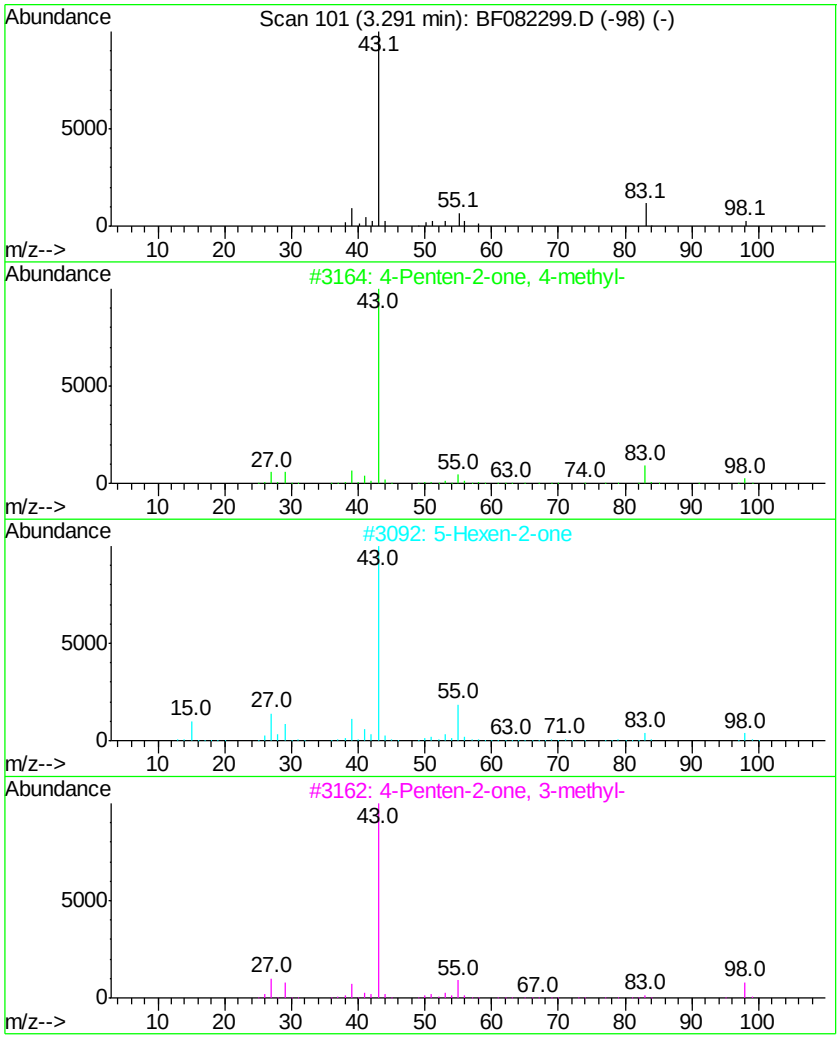
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

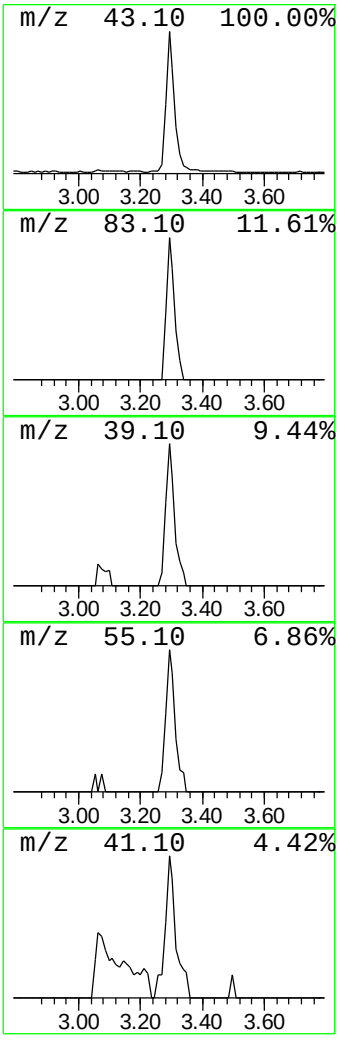
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	5.11 ng	111506	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	50
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	38
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	25
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





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Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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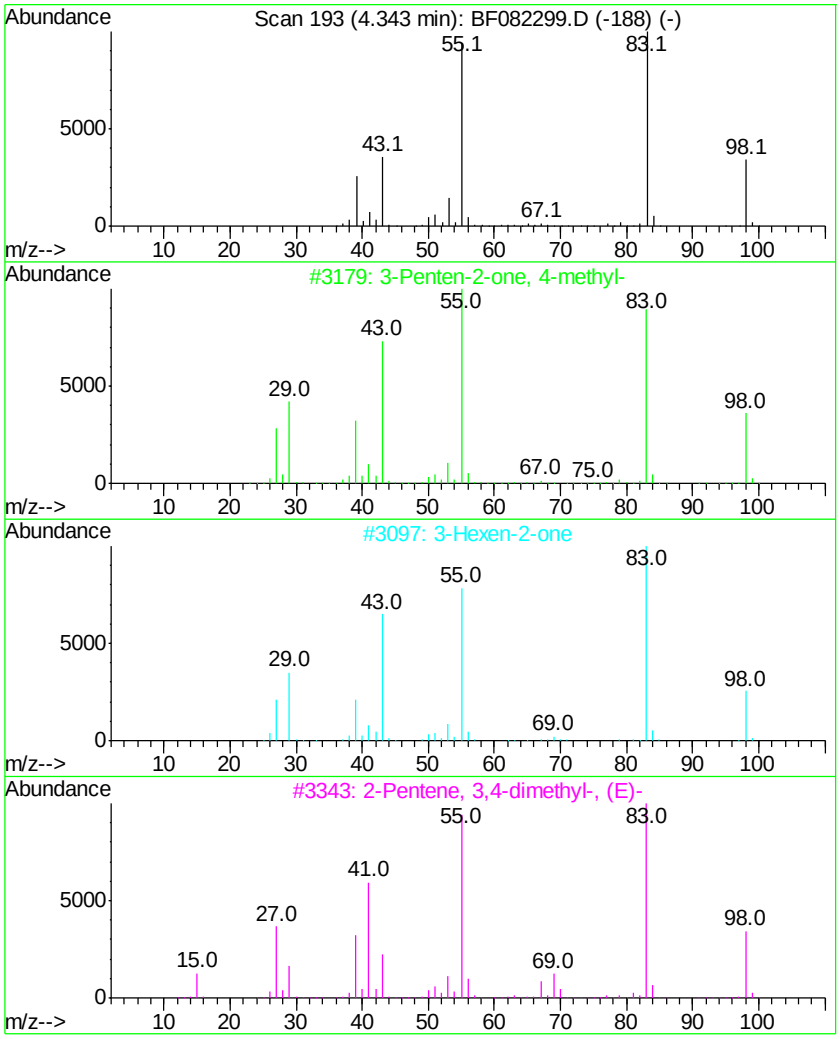
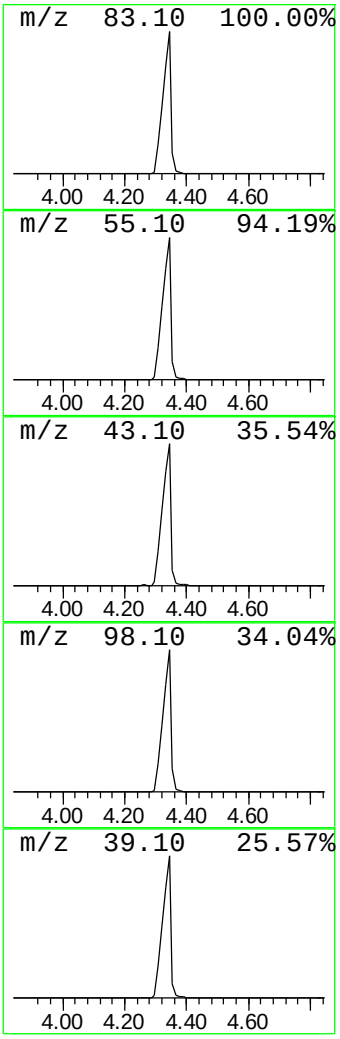
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	193.65 ng	4222940	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
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Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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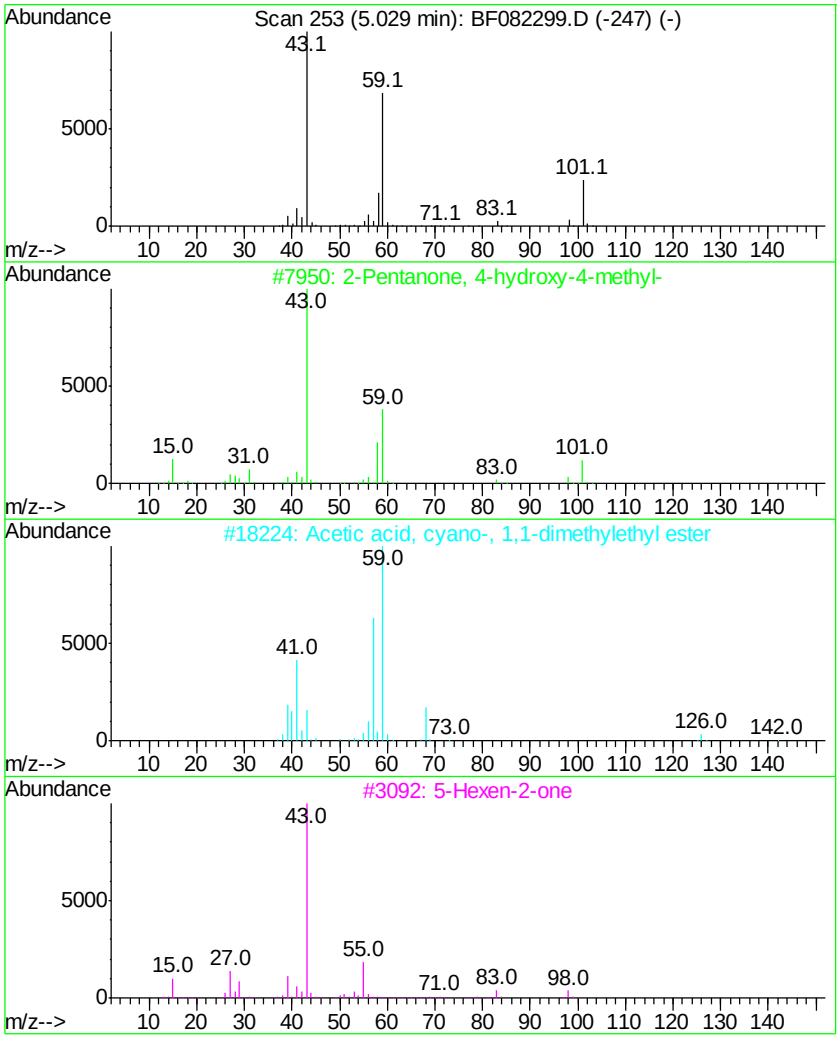
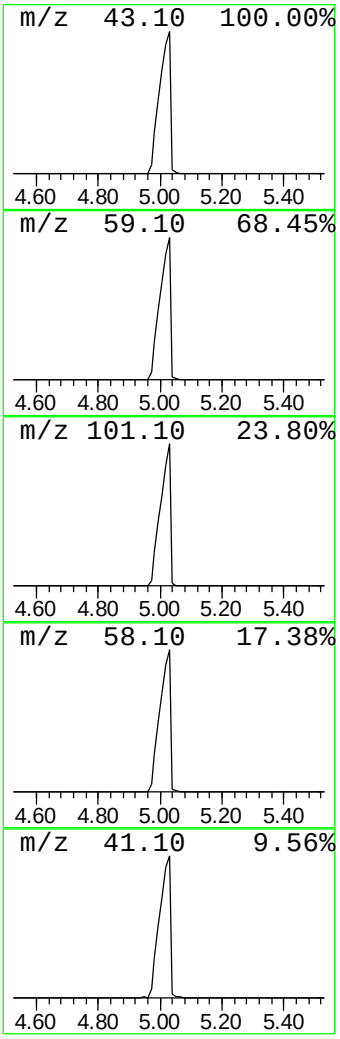
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	199.65 ng	4353860	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	72
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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
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Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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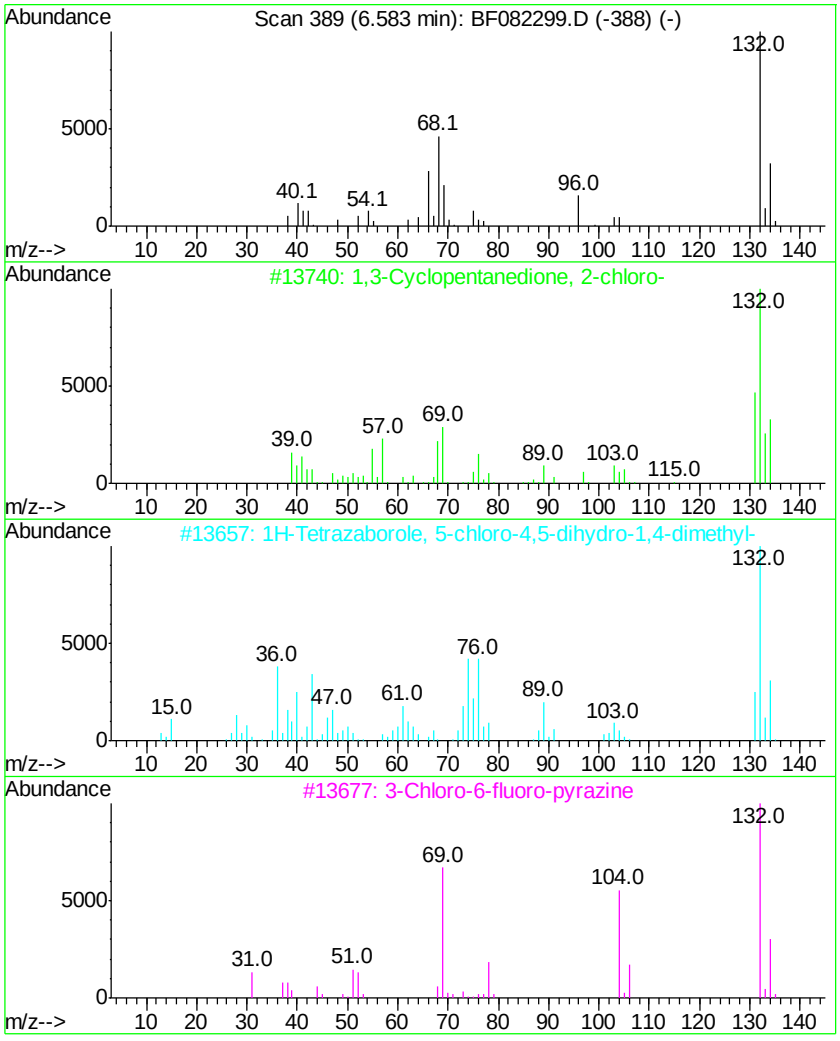
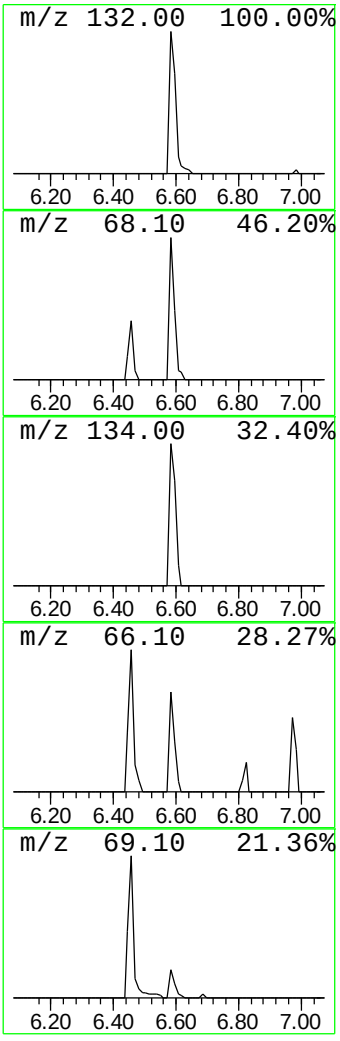
Peak Number 4 unknown6.58 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	2.39 ng	52153	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
2	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	16
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

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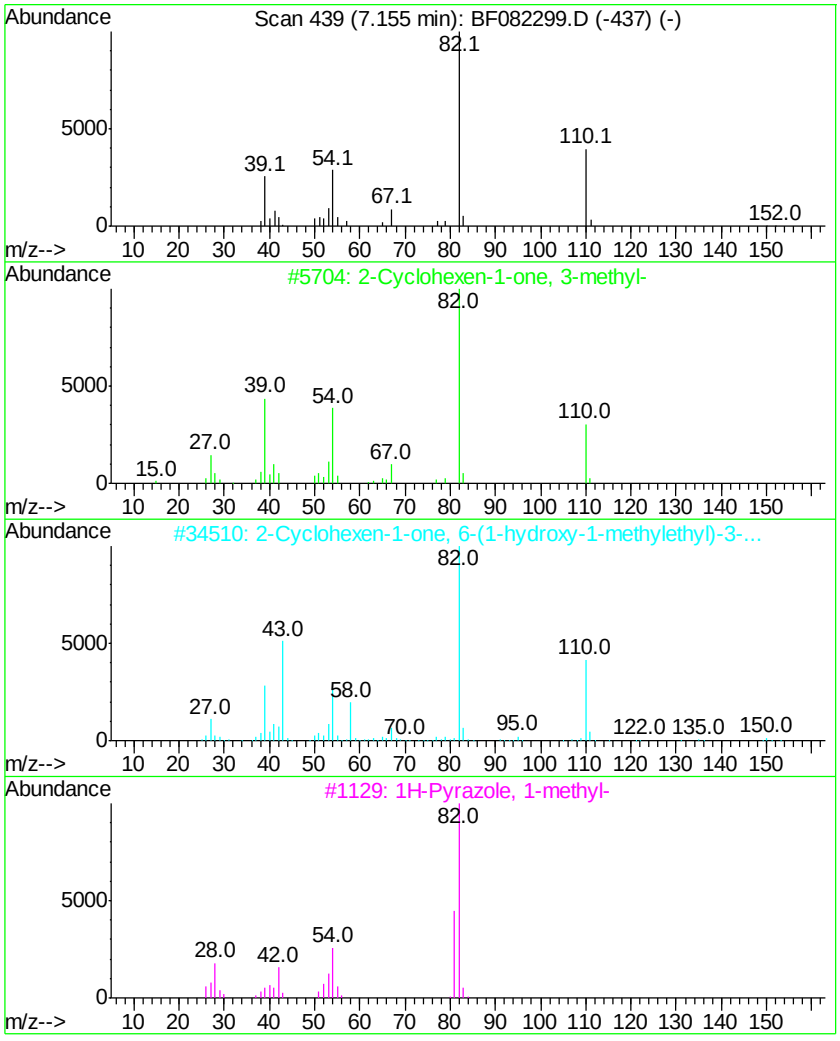
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

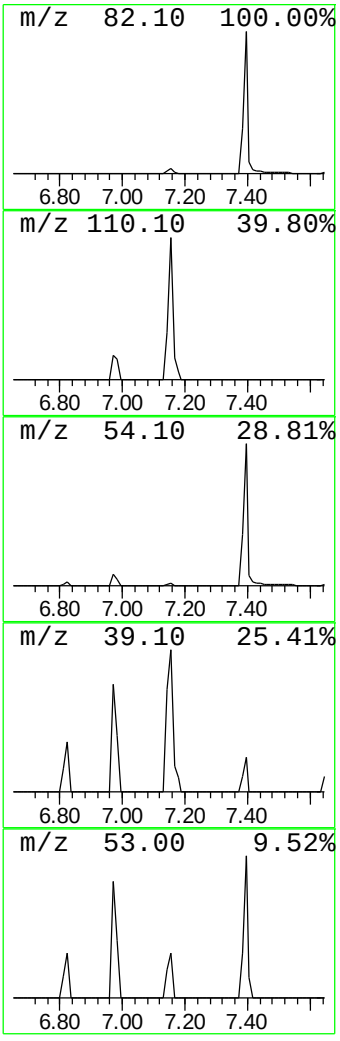
****

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	2.25 ng	49164	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
3	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	53
4	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	50
5	Azeleonitrile	150	C9H14N2	001675-69-0	50





Library Search Compound Report

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Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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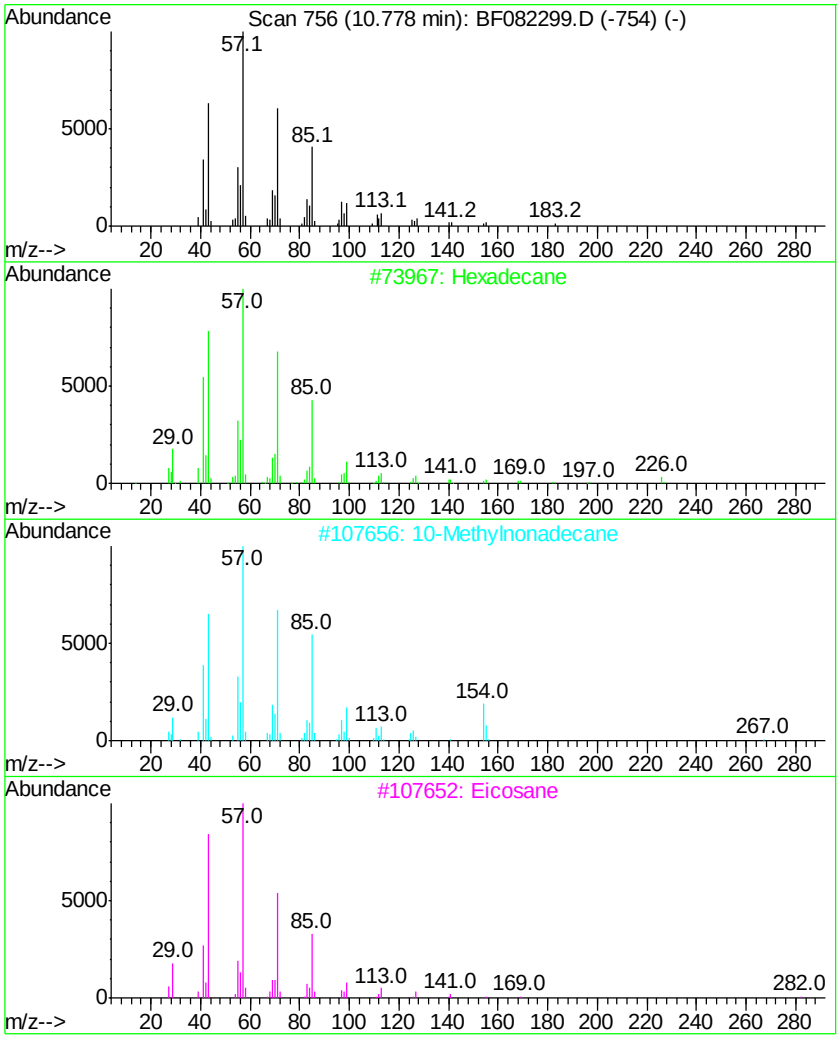
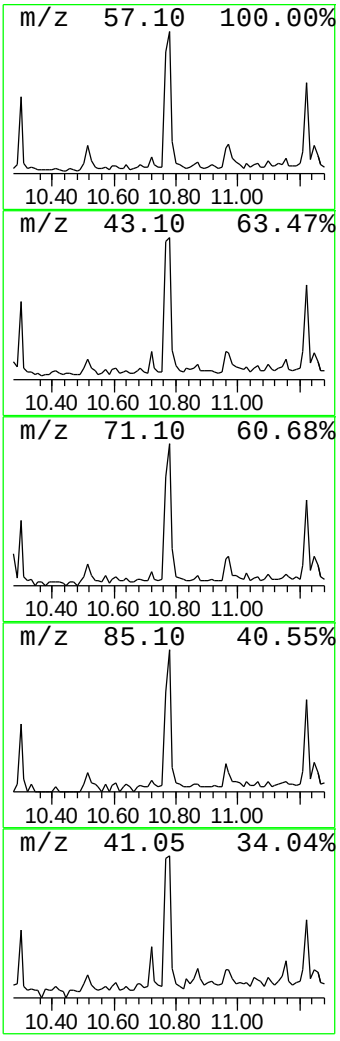
Peak Number 7 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	4.32 ng	160155	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	10-Methylnonadecane	282	C20H42	056862-62-5	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5	Nonadecane	268	C19H40	000629-92-5	86





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Sample : G4016-11
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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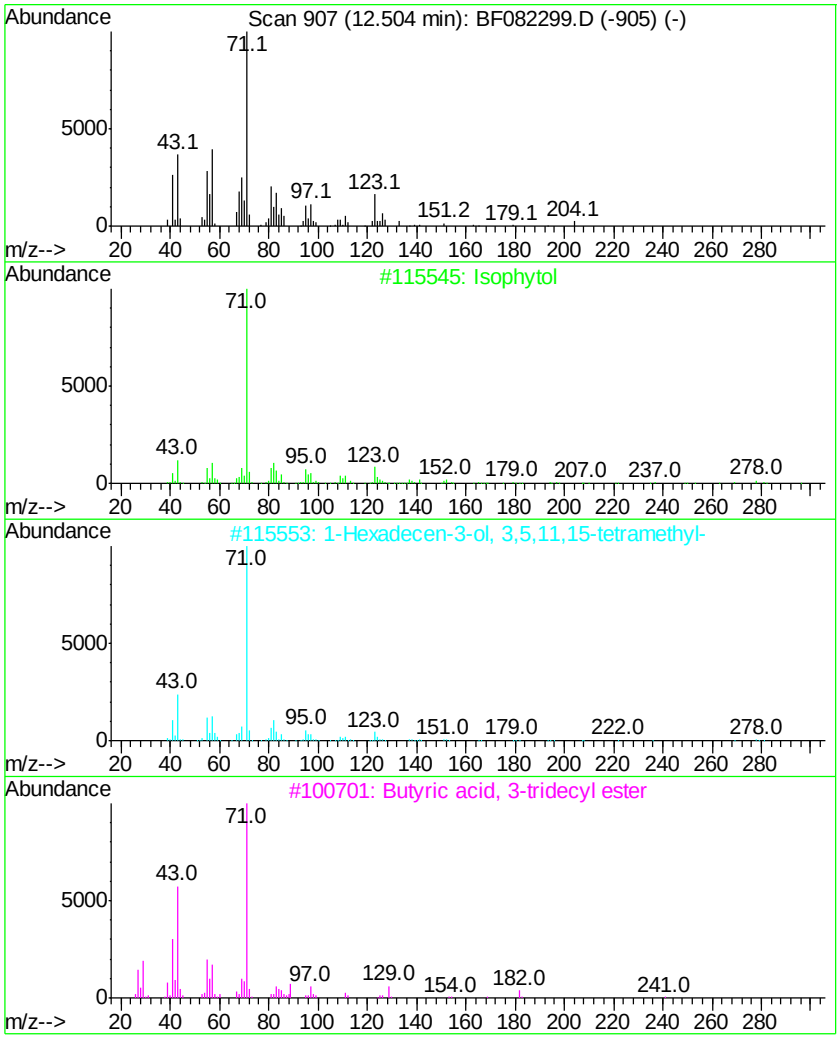
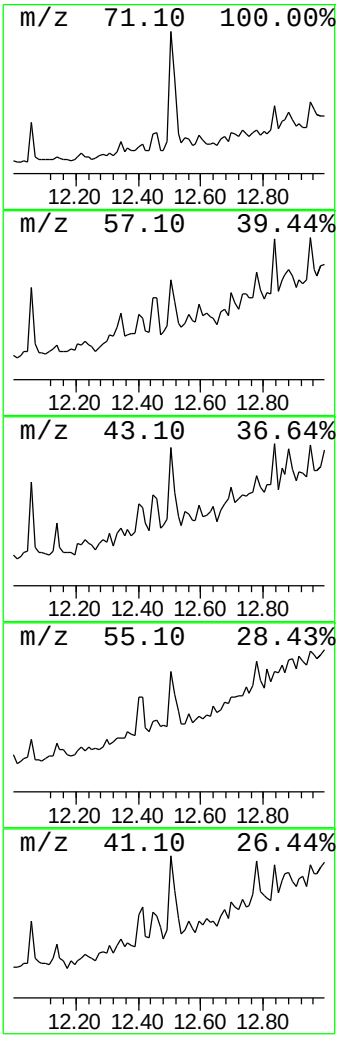
Peak Number 8 Isophytol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	2.22 ng	82309	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophytol	296	C20H40O	000505-32-8	64
2	1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	64
3	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	53
4	Phytol	296	C20H40O	000150-86-7	52
5	Heptan-2-ol, 5-(2-tetrahydrofurf...	200	C12H24O2	281676-71-9	50





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TIC Library : C:\DATABASE\NIST02.L
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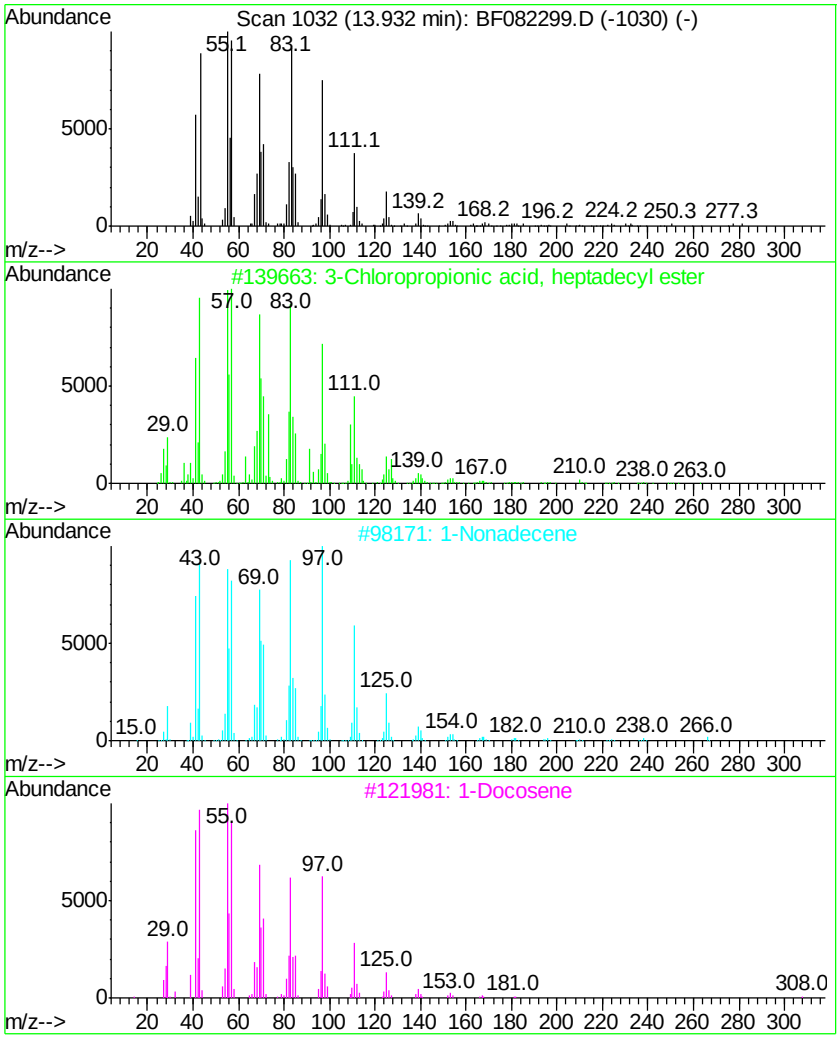
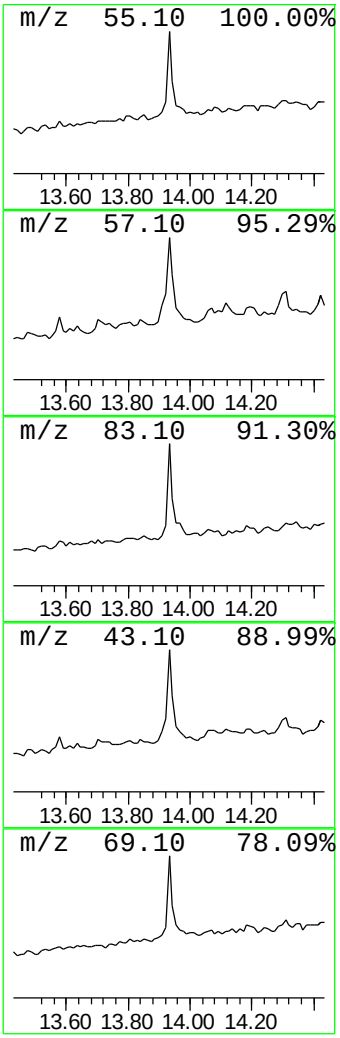
Peak Number 9 3-Chloropropionic acid, hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	13.11 ng	393248	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Docosene	308	C22H44	001599-67-3	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	87





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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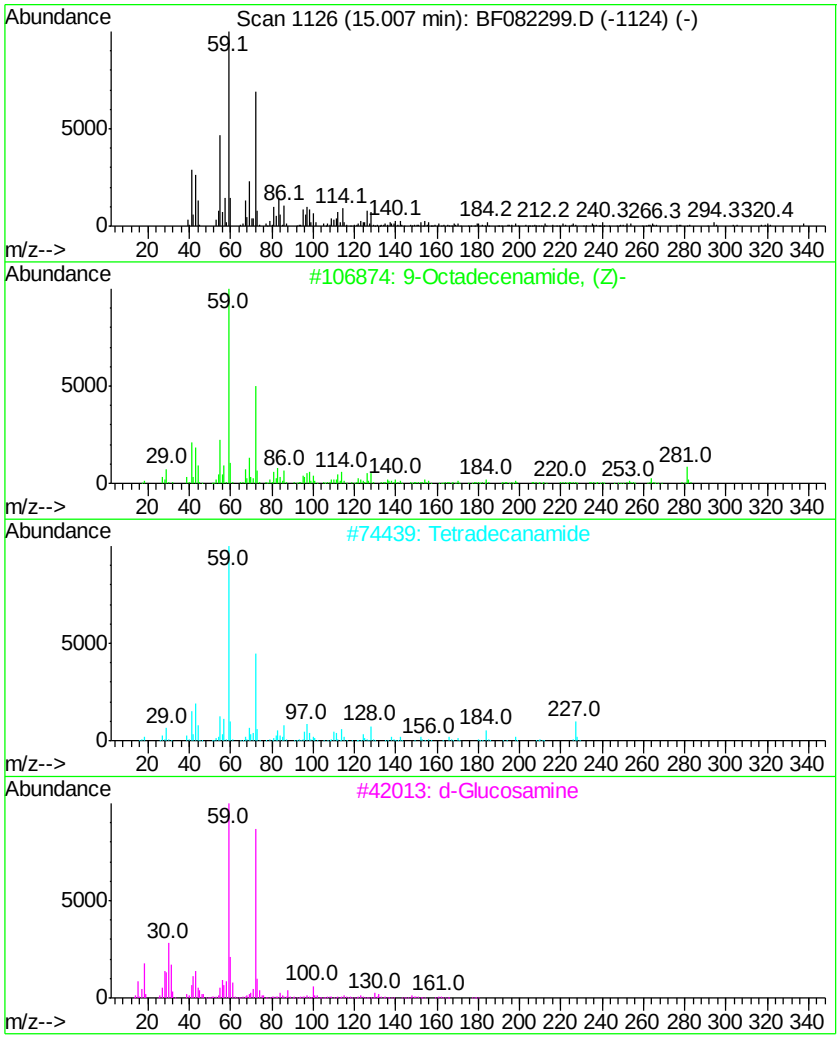
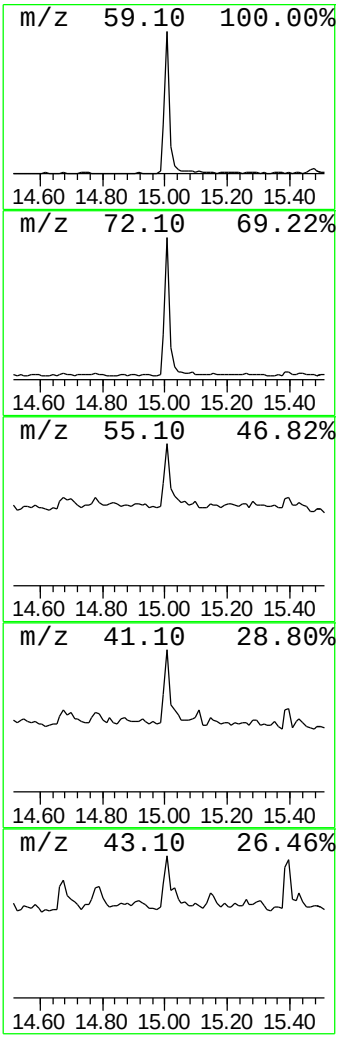
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	16.53 ng	347978	Perylene-d12	15.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	83
3	d-Glucosamine	179	C6H13NO5	000090-77-7	59
4	Decanamide-	171	C10H21NO	002319-29-1	59
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
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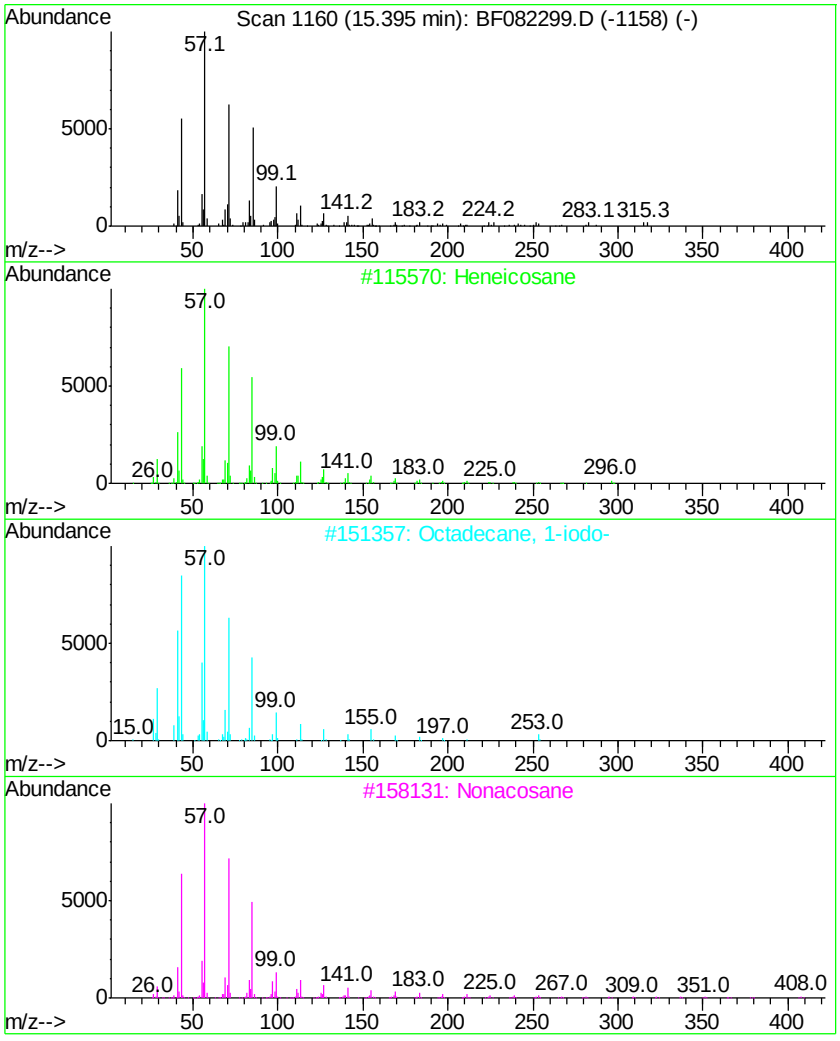
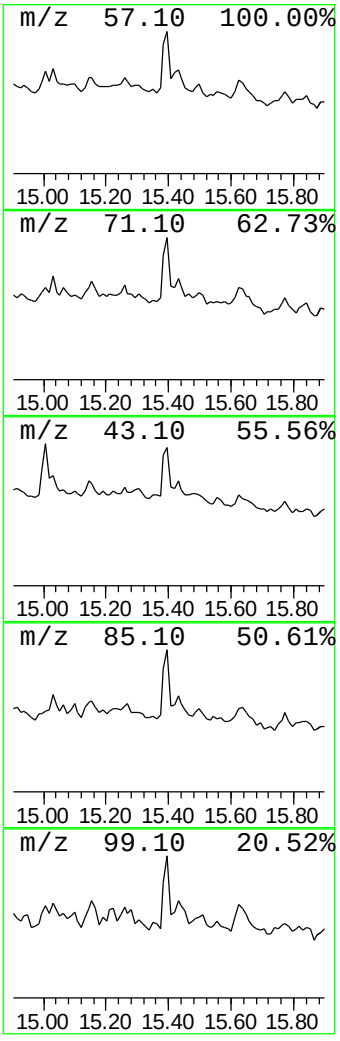
Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	5.84 ng	122859	Perylene-d12	15.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3	Nonacosane	408	C29H60	000630-03-5	80
4	Hexadecane	226	C16H34	000544-76-3	80
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80





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Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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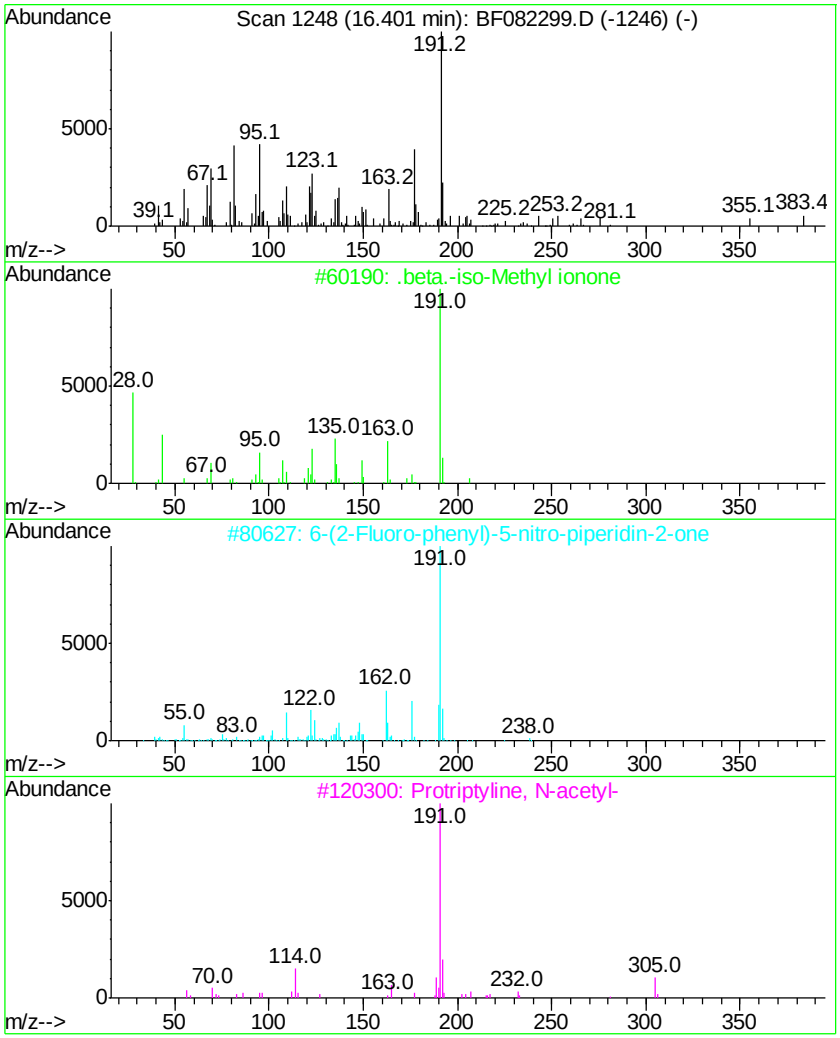
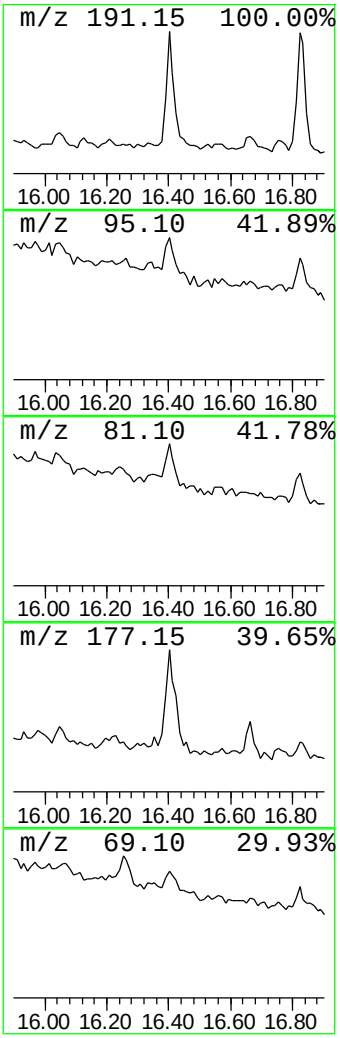
Peak Number 12 unknown16.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	15.94 ng	335543	Perylene-d12	15.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
2	6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	32
3	Protriptyline, N-acetyl-	305	C21H23NO	023047-28-1	27
4	5,5-Dimethyl-2-(2,2,2-trifluoro-...	249	C8H9F6NO	020967-43-5	27
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	25





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Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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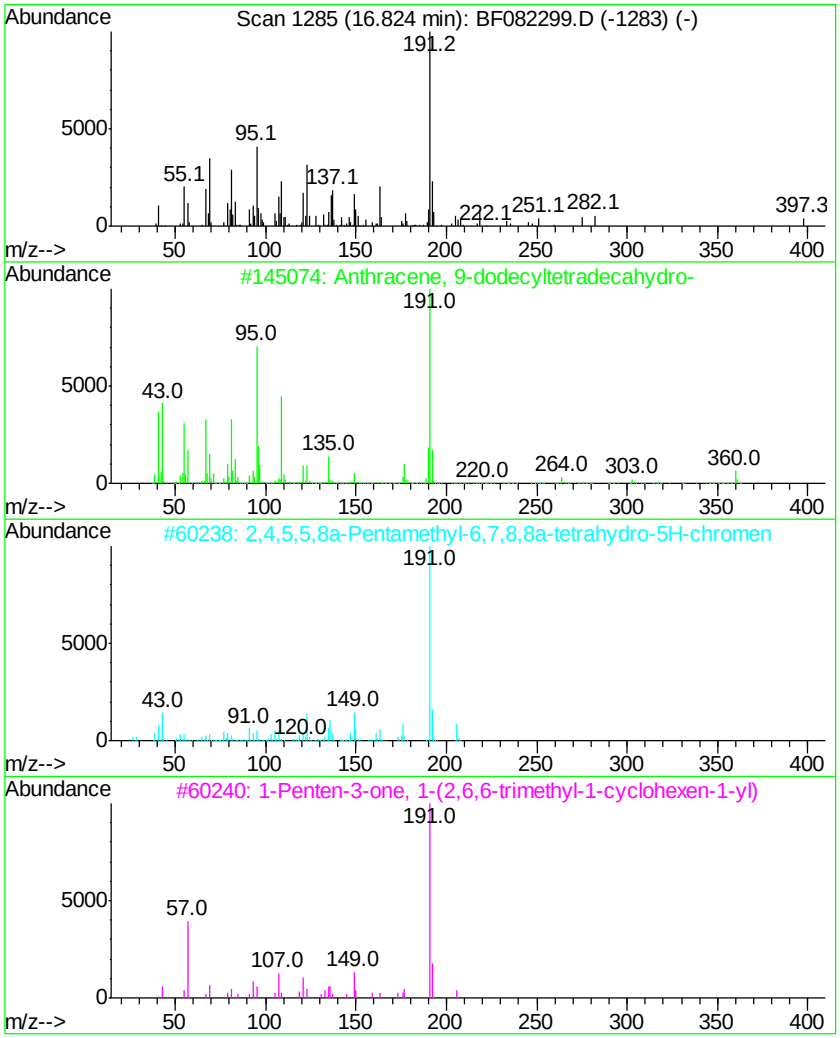
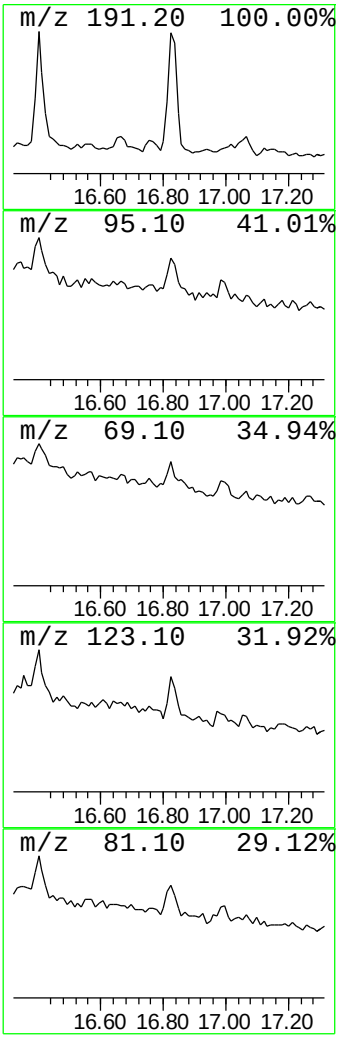
Peak Number 13 unknown16.82 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	10.82 ng	227731	Perylene-d12	15.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-dodecyltetradecahv...	360	C26H48	055401-75-7	38
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	38
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35
4	5H-Benzo[def]carbazole	191	C14H9N	000203-65-6	35
5	Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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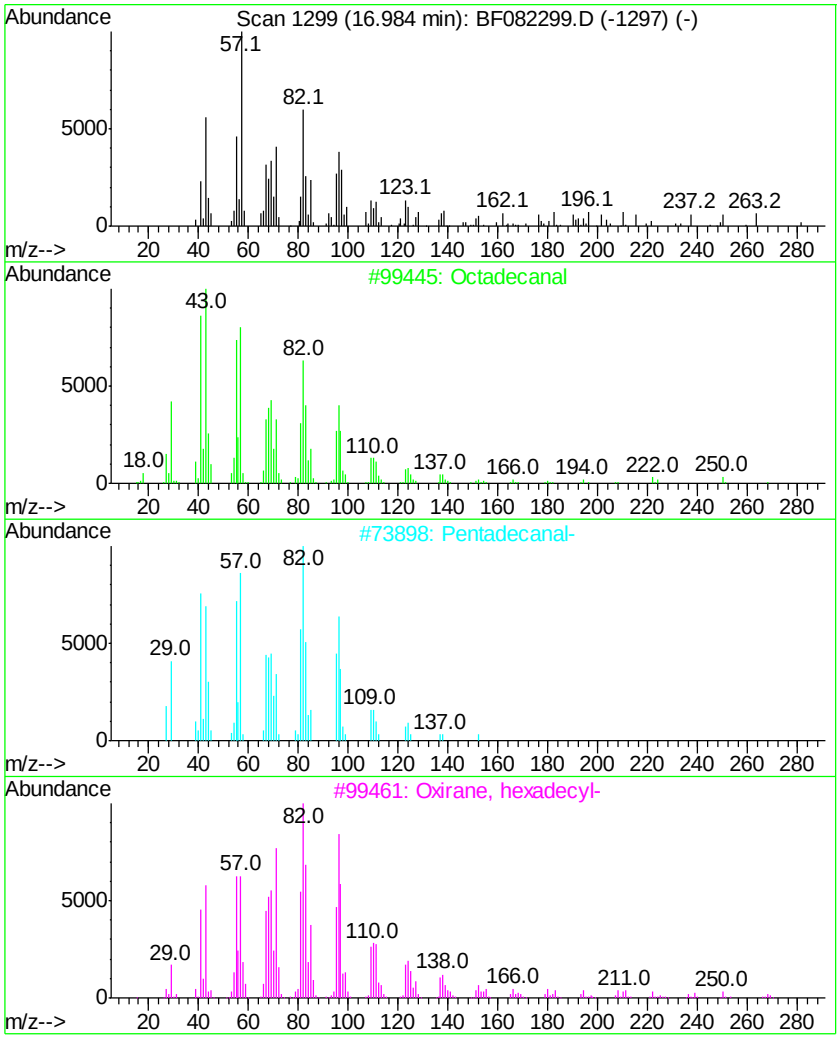
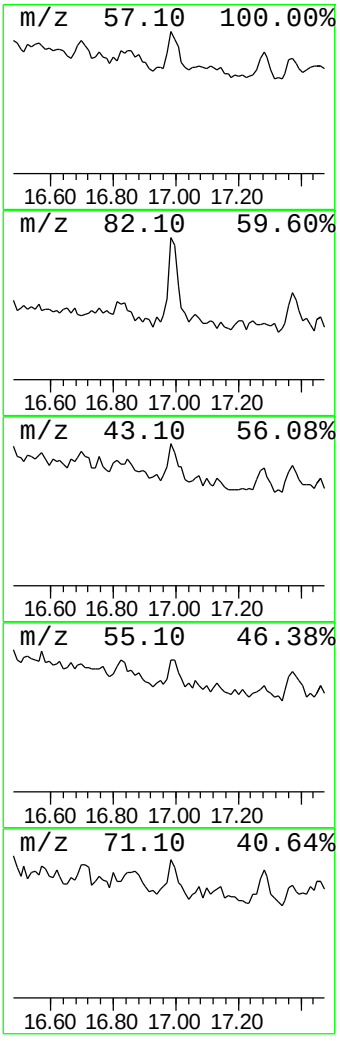
Peak Number 14 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	5.17 ng	108842	Perylene-d12	15.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	86
2	Pentadecanal-	226	C15H30O	002765-11-9	46
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	46
4	E-12-Octadecen-1-ol acetate	310	C20H38O2	1000130-93-6	45
5	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101615\
Data File : BF082299.D
Acq On : 15 Oct 2015 10:07
Operator : UM/IZ
Sample : G4016-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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
4-Penten-2-one, 4...	3.29	5.1	ng	111506	1	6.82	436150	20.0
3-Penten-2-one, 4...	4.34	193.7	ng	4222940	1	6.82	436150	20.0
2-Pentanone, 4-hy...	5.03	199.7	ng	4353860	1	6.82	436150	20.0
unknown6.58	6.58	2.4	ng	52153	1	6.82	436150	20.0
2-Cyclohexen-1-on...	7.15	2.3	ng	49164	1	6.82	436150	20.0
Hexadecane	10.78	4.3	ng	160155	4	11.36	742128	20.0
Isophytol	12.50	2.2	ng	82309	4	11.36	742128	20.0
3-Chloropropionic...	13.93	13.1	ng	393248	5	14.10	599761	20.0
9-Octadecenamide,...	15.01	16.5	ng	347978	6	15.72	421081	20.0
Heneicosane	15.40	5.8	ng	122859	6	15.72	421081	20.0
unknown16.40	16.40	15.9	ng	335543	6	15.72	421081	20.0
unknown16.82	16.82	10.8	ng	227731	6	15.72	421081	20.0
Octadecanal	16.98	5.2	ng	108842	6	15.72	421081	20.0