LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082296.D
Acq On : 15 Oct 2015 8:41
Operator : UM/IZ
Sample : G4016-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-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-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	3.303	98	102	111	rBV	65861	127716	2.20%	0.514%
2	4.354	188	194	197	rBV	2690803	5810225	100.00%	23.375%
3	5.029	247	253	256	rBV	1944692	4767749	82.06%	19.181%
4	5.634	304	306	308	rBV	58340	59709	1.03%	0.240%
5	6.457	375	378	383	rBV	94149	110712	1.91%	0.445%
6	6.823	408	410	412	rBV	457421	438086	7.54%	1.762%
7	6.972	421	423	426	rBV	1052196	1393696	23.99%	5.607%
8	7.155	437	439	444	rVB	49008	66206	1.14%	0.266%
9	7.395	457	460	462	rBV	1070240	1099930	18.93%	4.425%
10	8.115	520	523	525	rBV	536587	599246	10.31%	2.411%
11	9.189	615	617	620	rBV	2095930	2125841	36.59%	8.552%
12	9.589	649	652	654	rBV	455712	381775	6.57%	1.536%
13	9.863	674	676	679	rBV	522346	738355	12.71%	2.970%
14	10.766	754	755	760	rVB	85459	129374	2.23%	0.520%
15	10.984	772	774	776	rBV	217123	239433	4.12%	0.963%
16	11.361	804	807	809	rBV	740743	741715	12.77%	2.984%
17	12.401	896	898	901	rBV	80442	103674	1.78%	0.417%
18	12.961	944	947	949	rBV	2283756	2496257	42.96%	10.043%
19	13.178	964	966	969	rBV2	70710	114930	1.98%	0.462%
20	13.852	1022	1025	1027	rBV	724047	775236	13.34%	3.119%
21	13.887	1027	1028	1036	rVB	259142	419748	7.22%	1.689%
22	14.058	1041	1043	1046	rBV	518989	612053	10.53%	2.462%
23	14.915	1115	1118	1122	rBV	363831	541601	9.32%	2.179%
24	15.613	1176	1179	1186	rVB	364632	613411	10.56%	2.468%
25	16.287	1236	1238	1242	rVB2	66542	141064	2.43%	0.568%
26	16.710	1272	1275	1283	rVB3	75848	208865	3.59%	0.840%

Sum of corrected areas: 24856607

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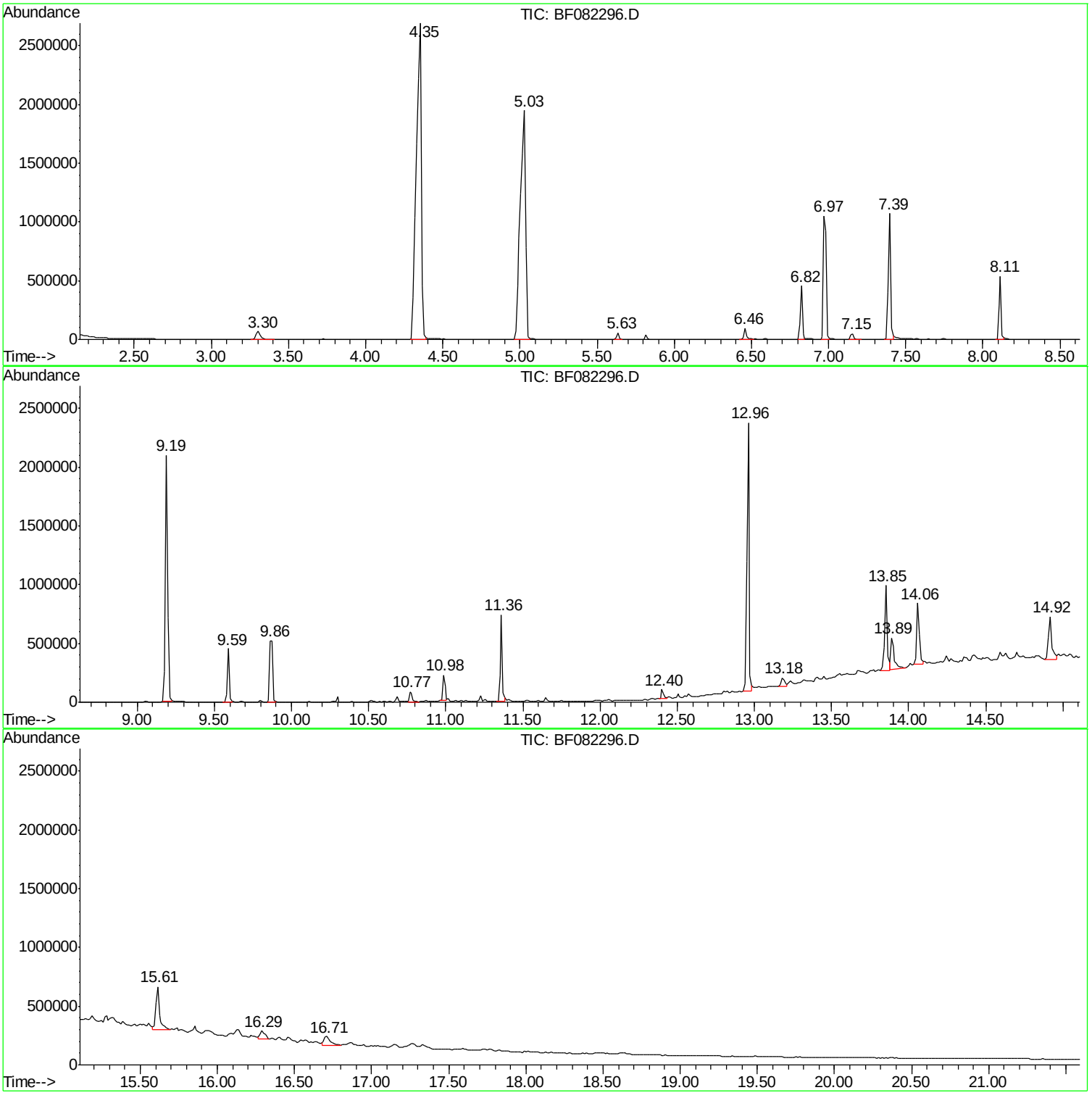
ClientSampleId : CS-8

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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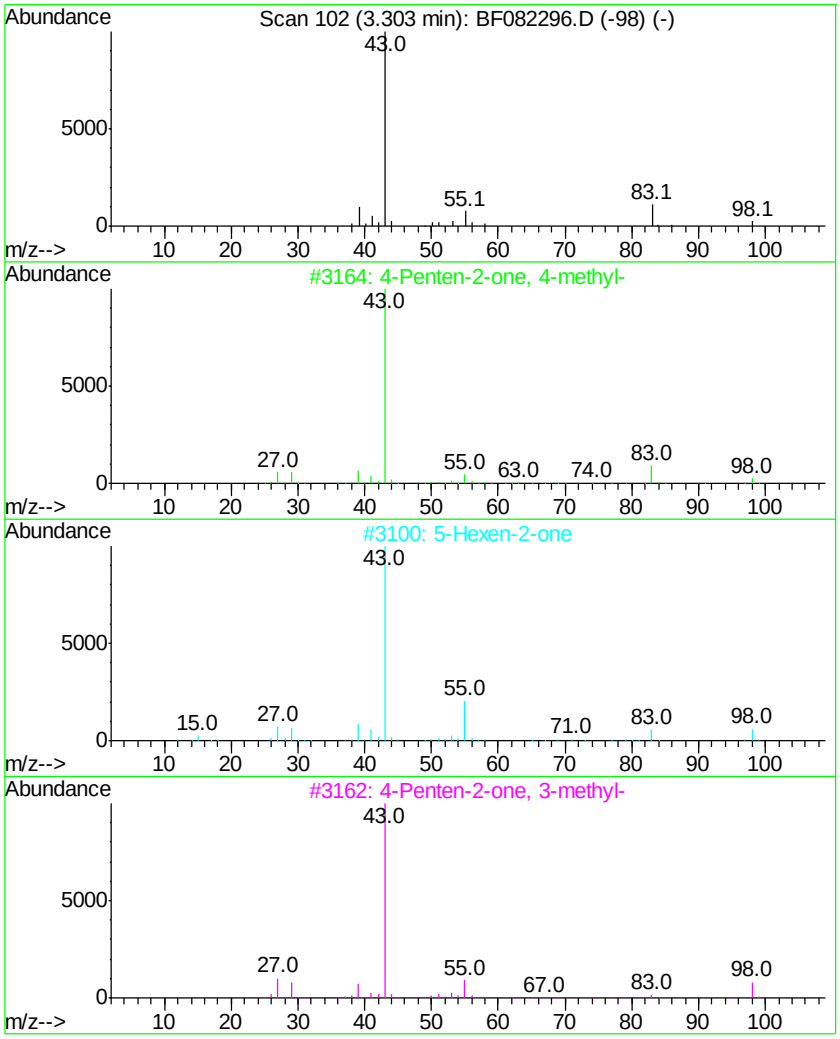
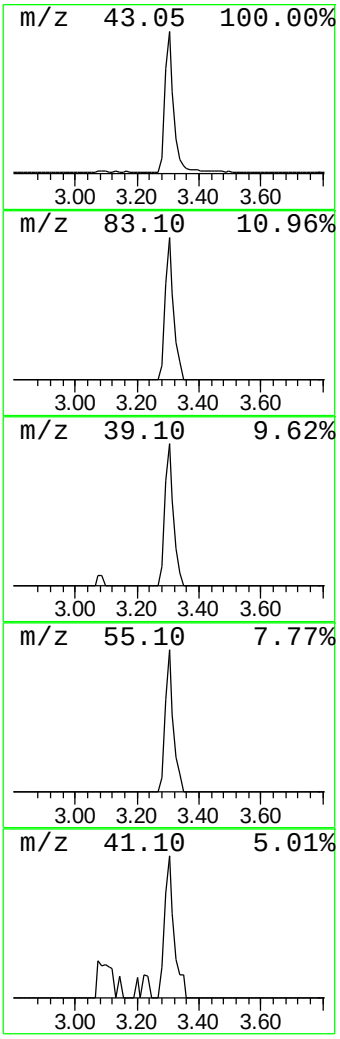
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	5.83 ng	127716	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	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	33
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9





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ClientSampleId : CS-8

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TIC Integration Parameters: LSCINT.P

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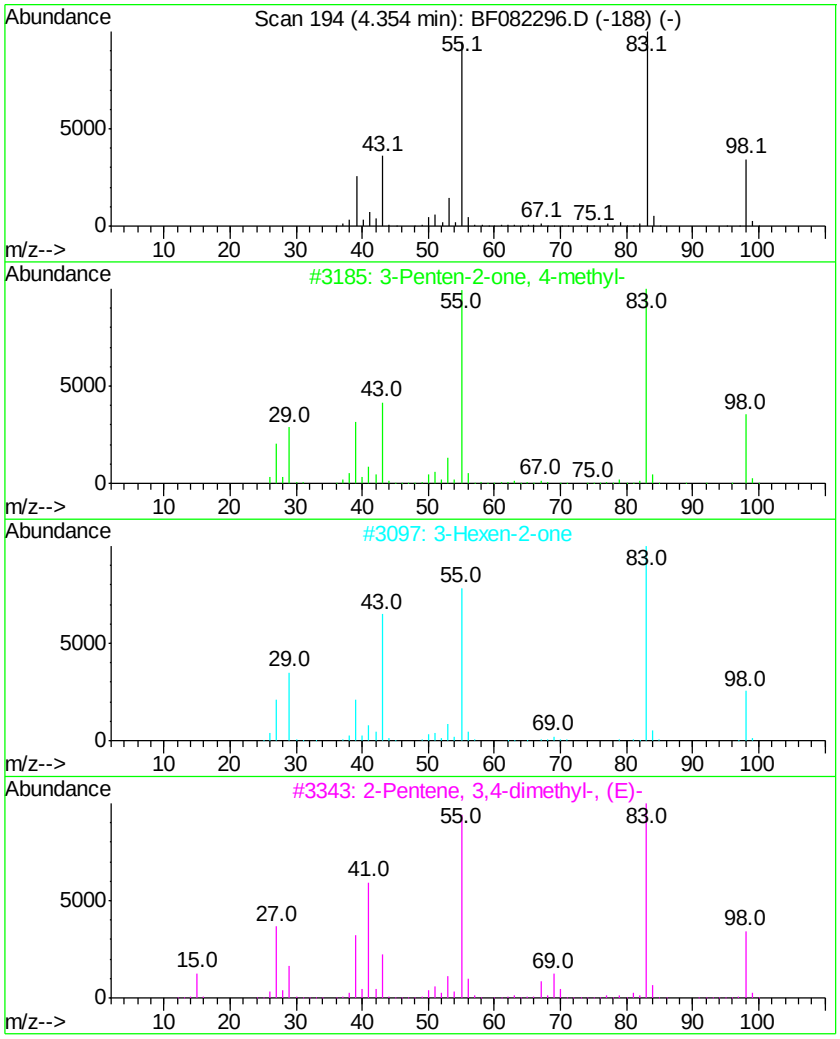
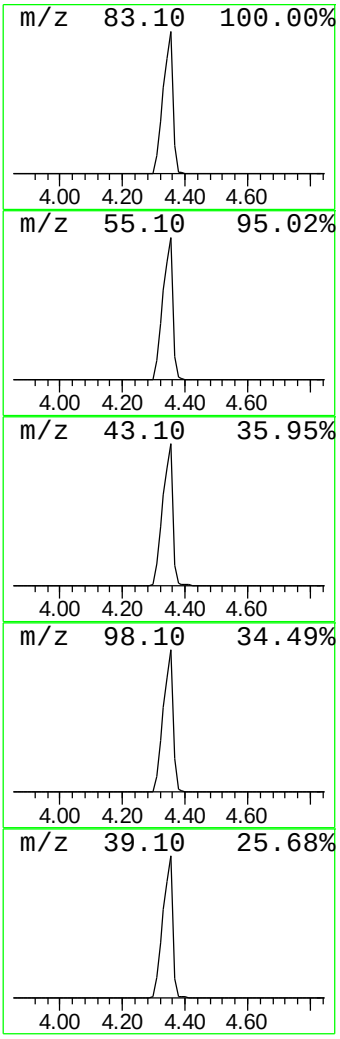
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	265.26 ng	5810230	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	94
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Sample : G4016-07
Misc :
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Instrument : BNA_F
ClientSampleId : CS-8

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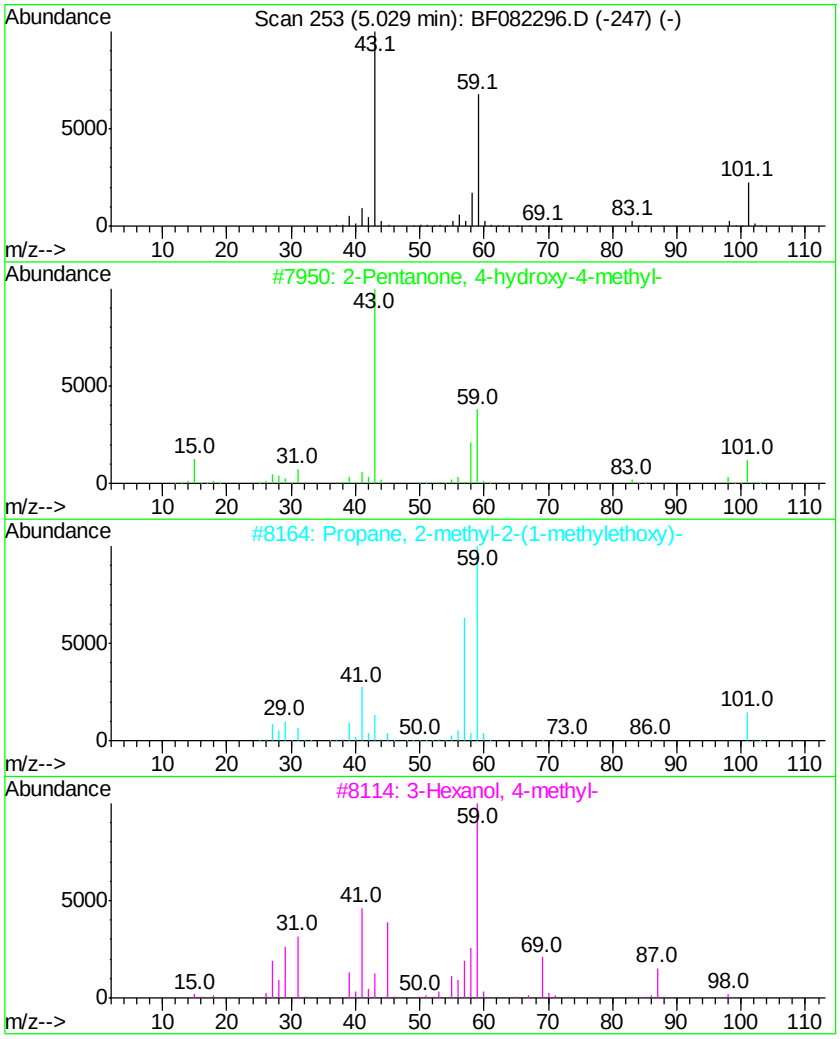
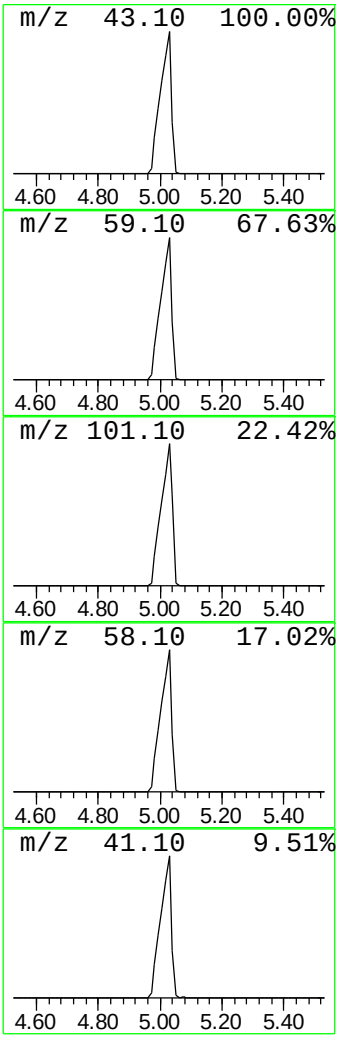
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	217.66 ng	4767750	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	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : CS-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Integration Parameters: LSCINT.P

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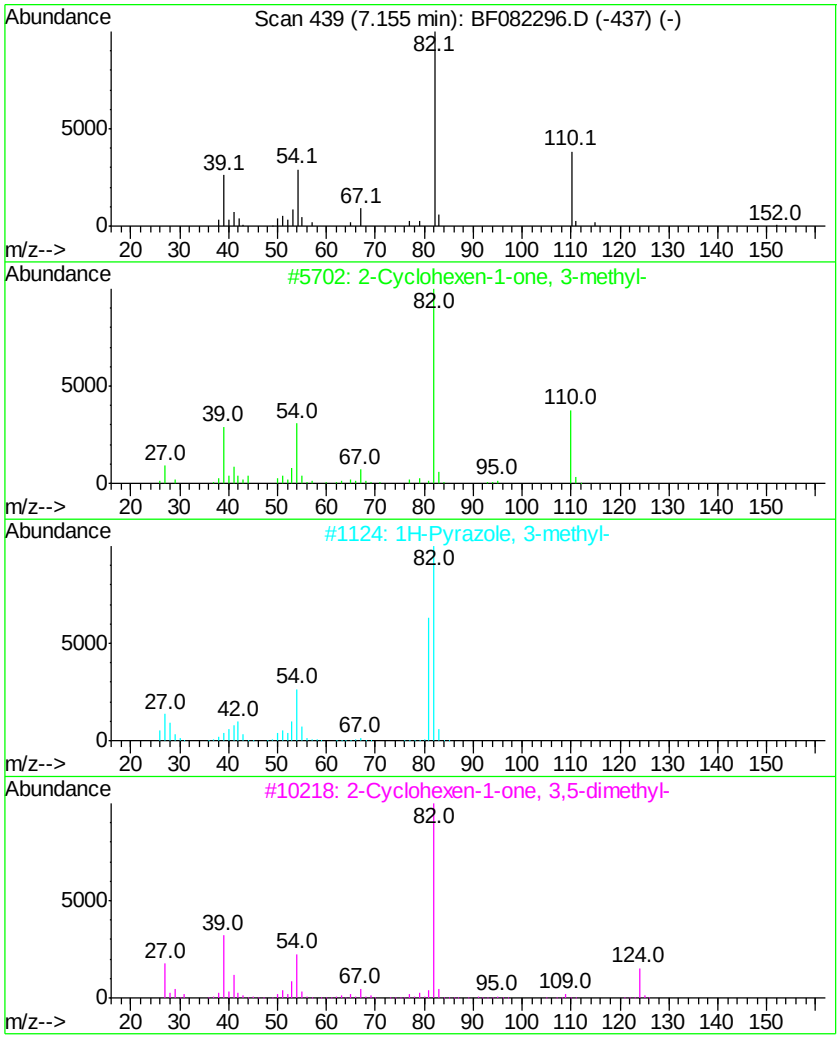
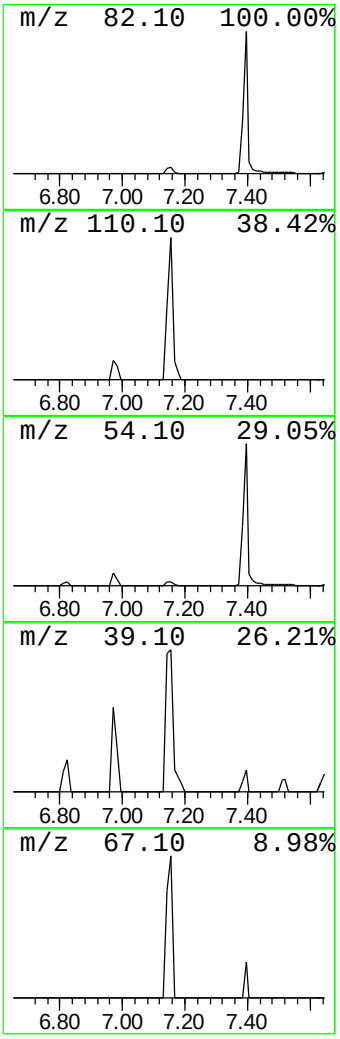
Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	3.02 ng	66206	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	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	53
3	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	53
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	40
5	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	40





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Sample : G4016-07
Misc :
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Instrument : BNA_F
ClientSampleId : CS-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
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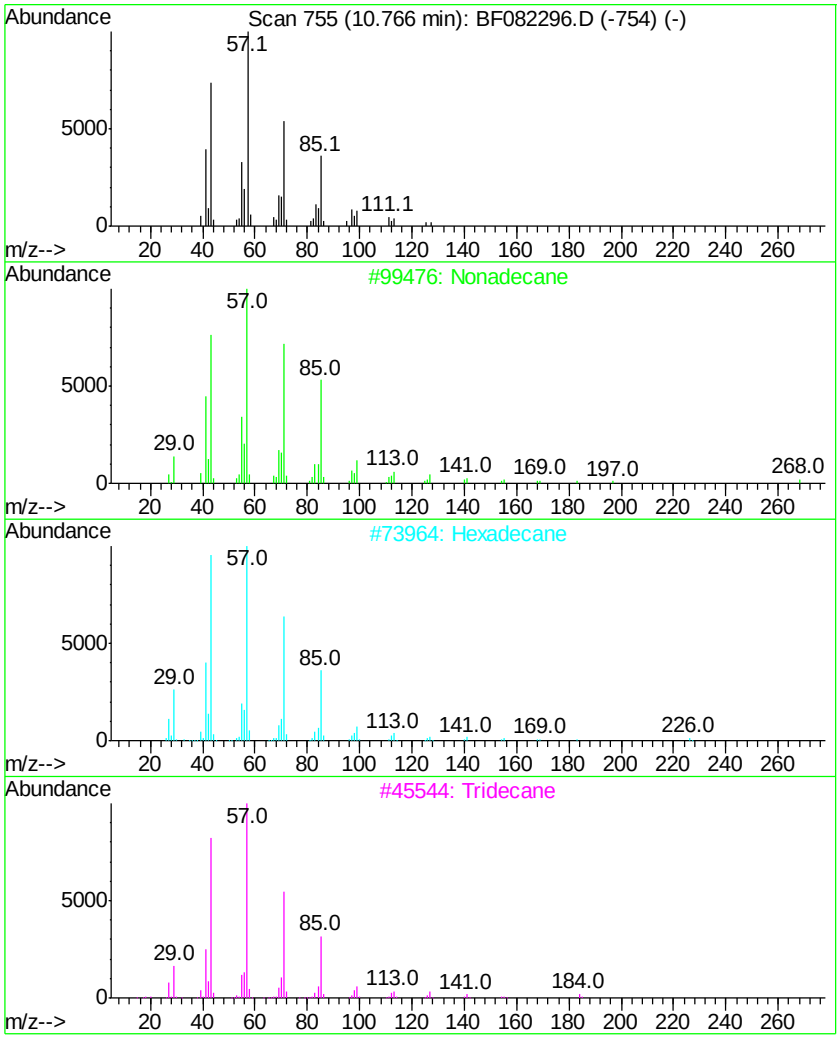
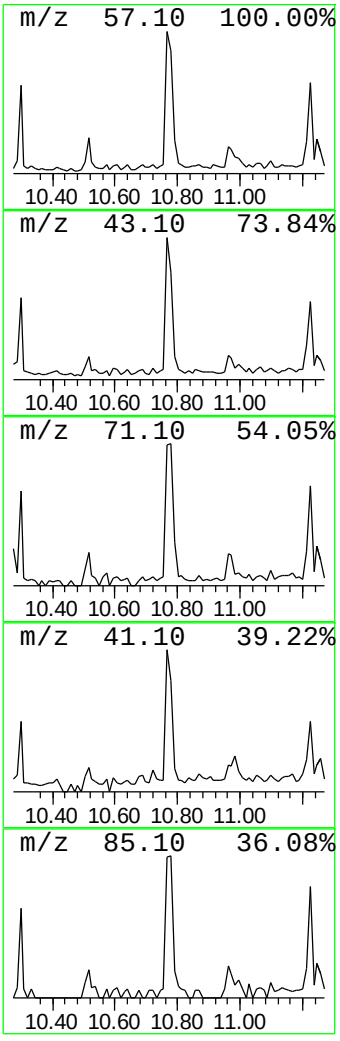
Peak Number 7 Nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	3.49 ng	129374	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexadecane	226	C16H34	000544-76-3	80
3	Tridecane	184	C13H28	000629-50-5	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	Eicosane	282	C20H42	000112-95-8	72





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Misc :
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Instrument : BNA_F
ClientSampleId : CS-8

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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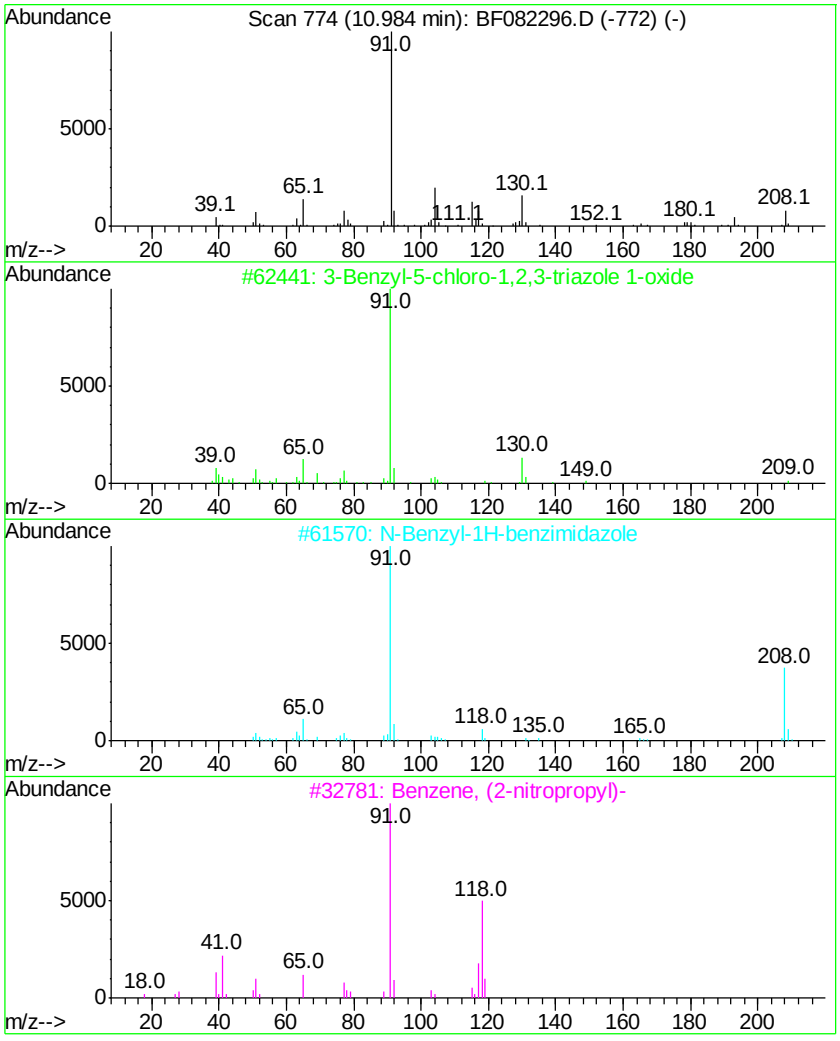
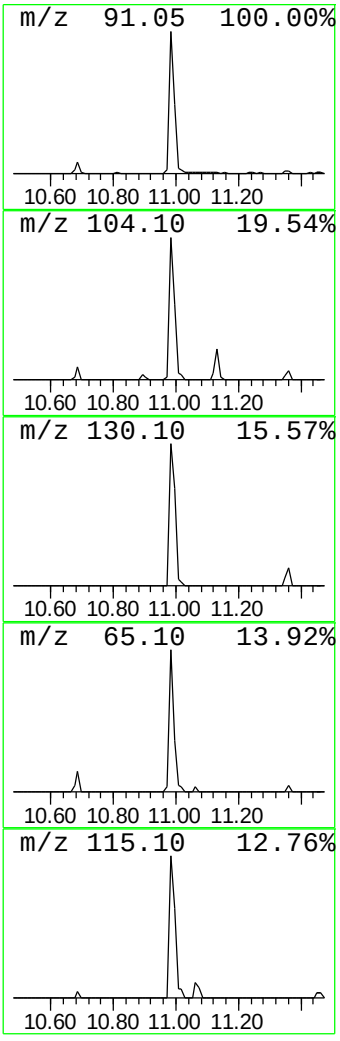
Peak Number 8 unknown10.98 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	6.46 ng	239433	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Benzyl-5-chloro-1,2,3-triazole...	209	C9H8ClN3O	116932-67-3	46
2	N-Benzyl-1H-benzimidazole	208	C14H12N2	004981-92-4	38
3	Benzene, (2-nitropropyl)-	165	C9H11NO2	017322-34-8	35
4	Bicyclo[3.1.0]hex-2-ene, 4-methy...	134	C10H14	036262-09-6	35
5	1,2-Diphenyl-1-isocyanoethane	207	C15H13N	003128-88-9	35





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

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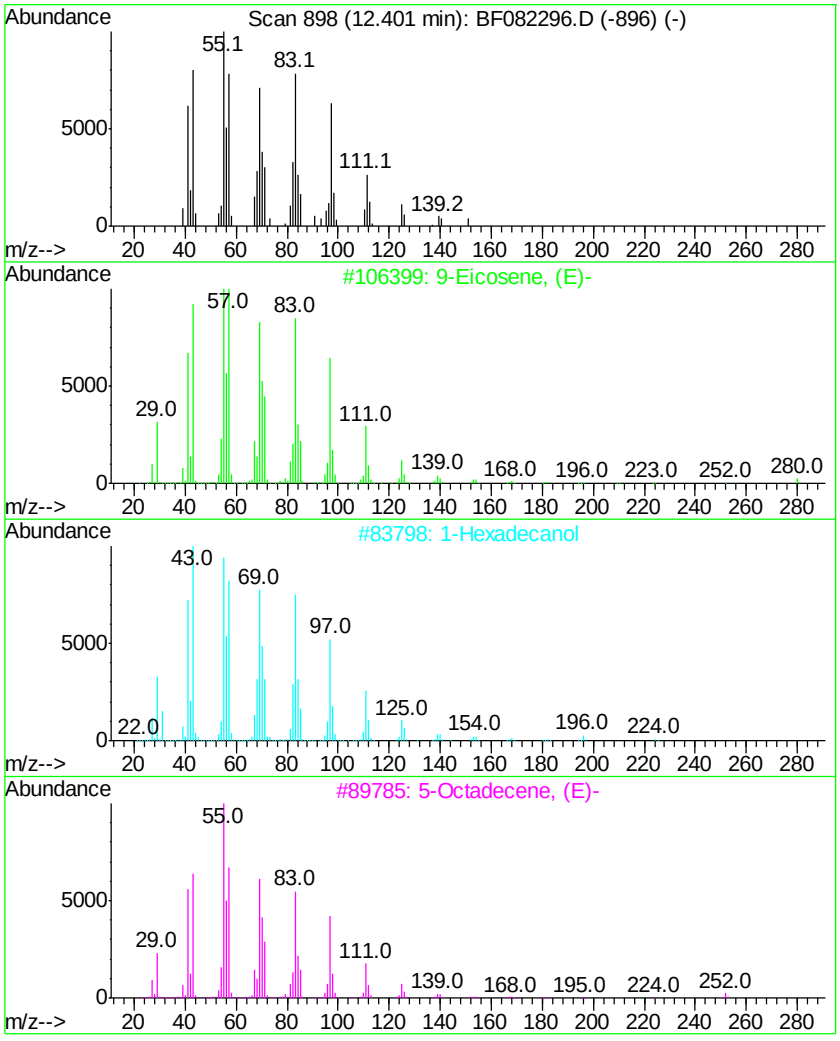
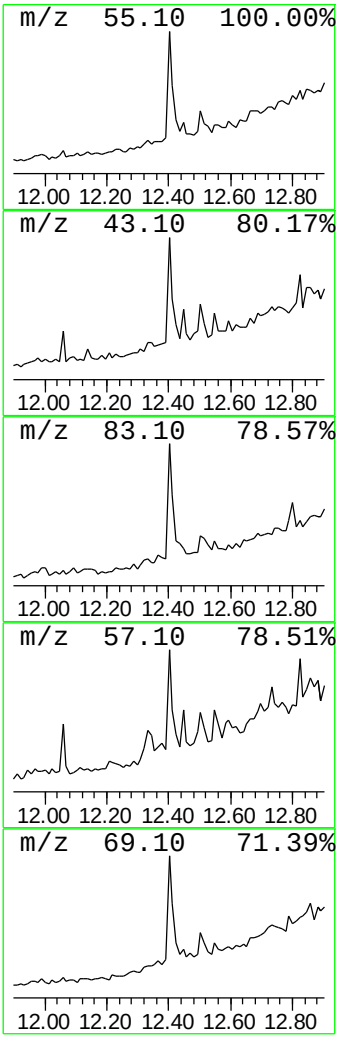
Peak Number 9 9-Eicosene, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	2.80 ng	103674	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	91
5	1-Heptadecanol	256	C17H36O	001454-85-9	90





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TIC Library : C:\DATABASE\NIST02.L
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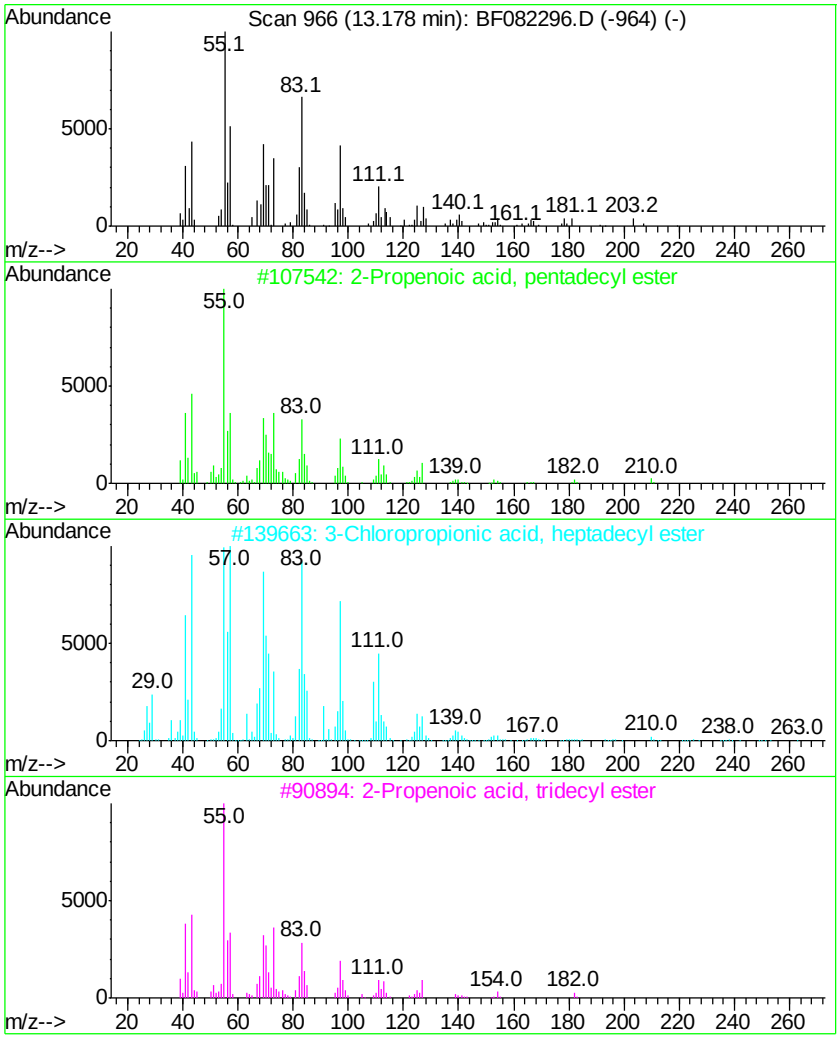
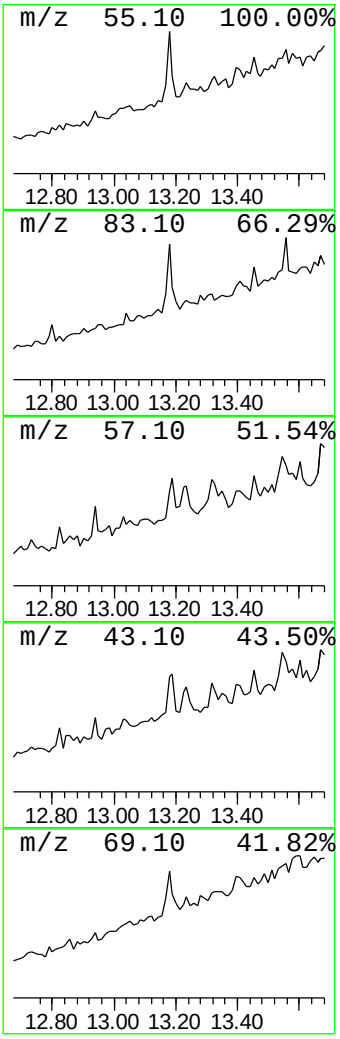
****

Peak Number 10 2-Propenoic acid, pentadecy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	3.76 ng	114930	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, pentadecyl ester	282	C18H34O2	043080-23-5	64
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	46
3	2-Propenoic acid, tridecyl ester	254	C16H30O2	003076-04-8	43
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38
5	1-Octadecene	252	C18H36	000112-88-9	30





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

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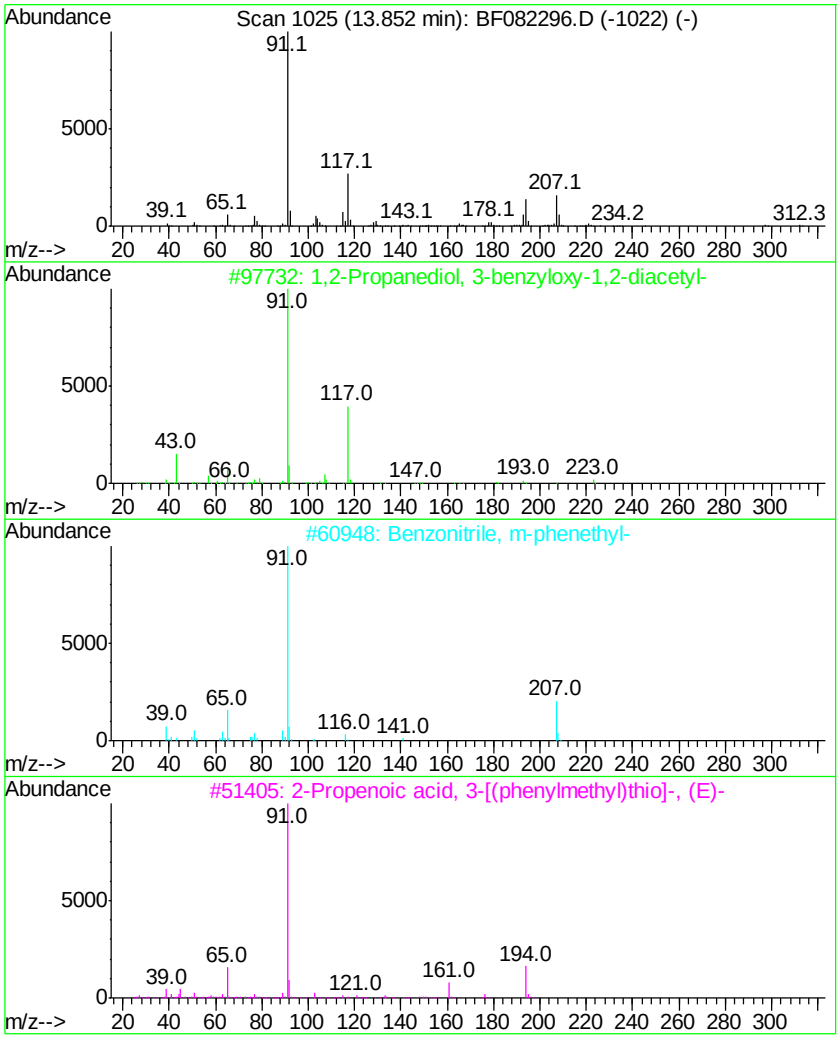
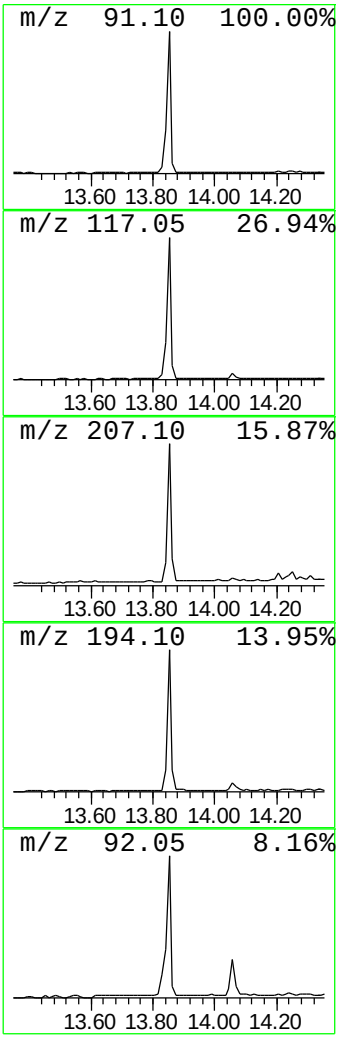
Peak Number 11 unknown13.85 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	25.33 ng	775236	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Propanediol, 3-benzyloxy-1,2...	266	C14H18O5	013754-10-4	32
2	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	25
3	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	17
4	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
5	Alpha-phenyl-alpha-tropylacetald...	378	C22H22N2O2S	022532-16-7	16





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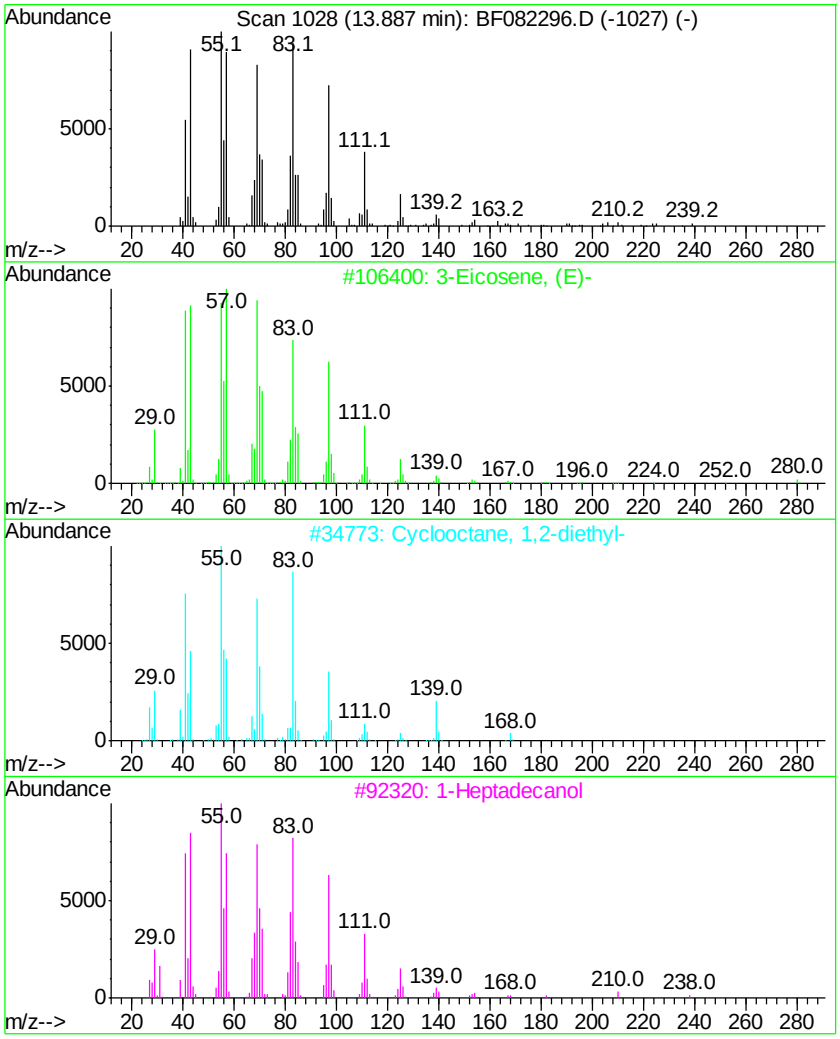
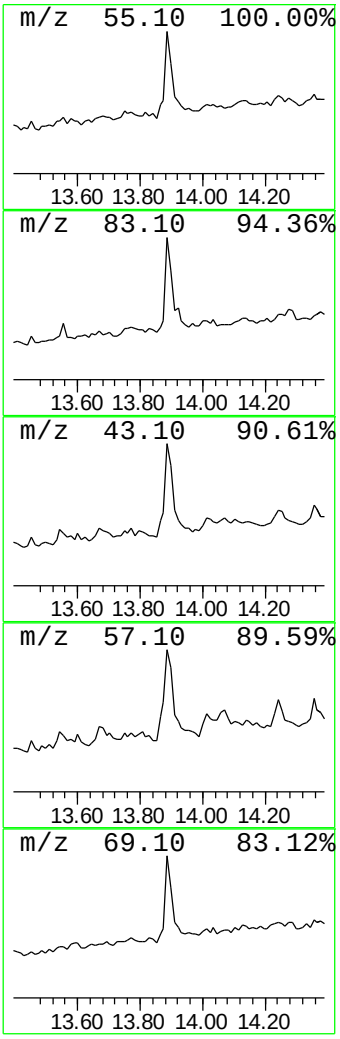
****

Peak Number 12 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	13.72 ng	419748	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
2	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	87
3	1-Heptadecanol	256	C17H36O	001454-85-9	83
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	74
5	1-Hexadecanol	242	C16H34O	036653-82-4	74





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Data File : BF082296.D
Acq On : 15 Oct 2015 8:41
Operator : UM/IZ
Sample : G4016-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-8

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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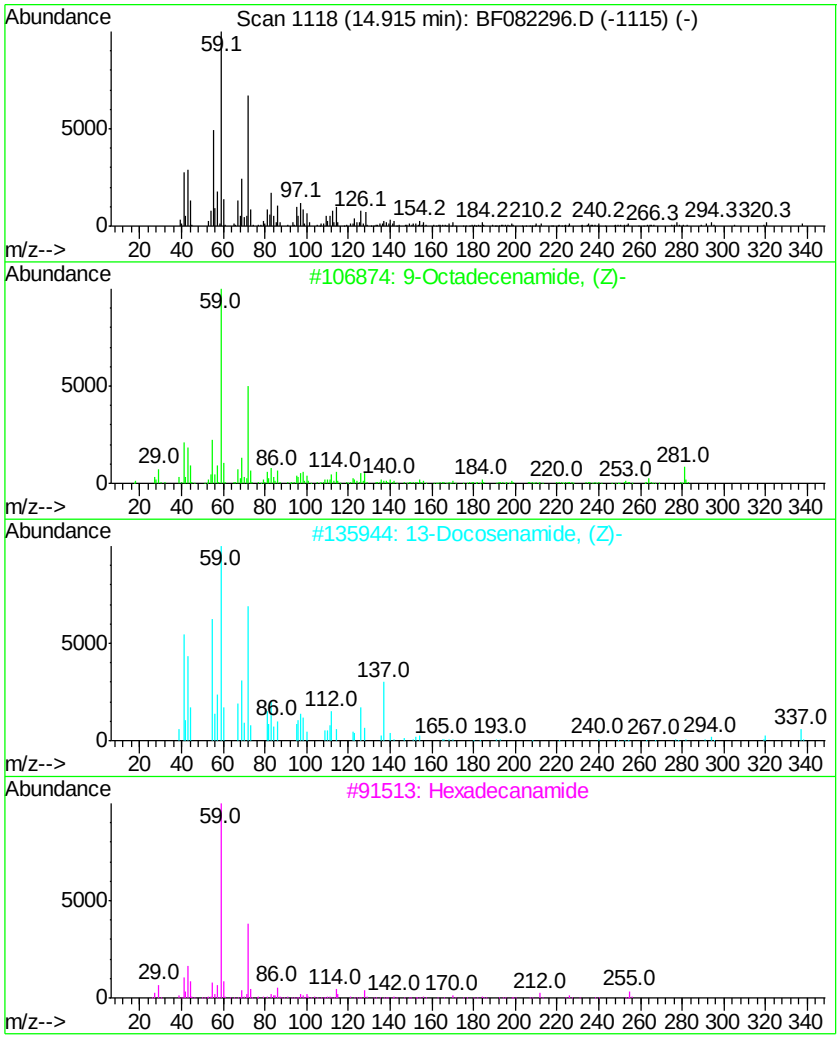
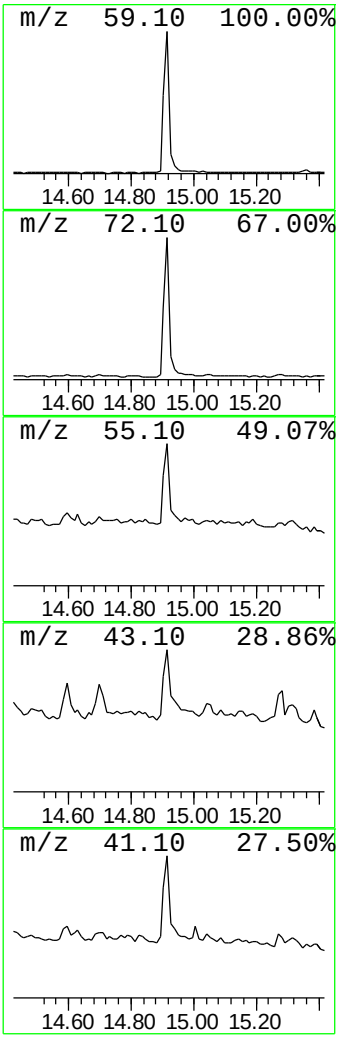
Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	17.66 ng	541601	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082296.D
Acq On : 15 Oct 2015 8:41
Operator : UM/IZ
Sample : G4016-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-8

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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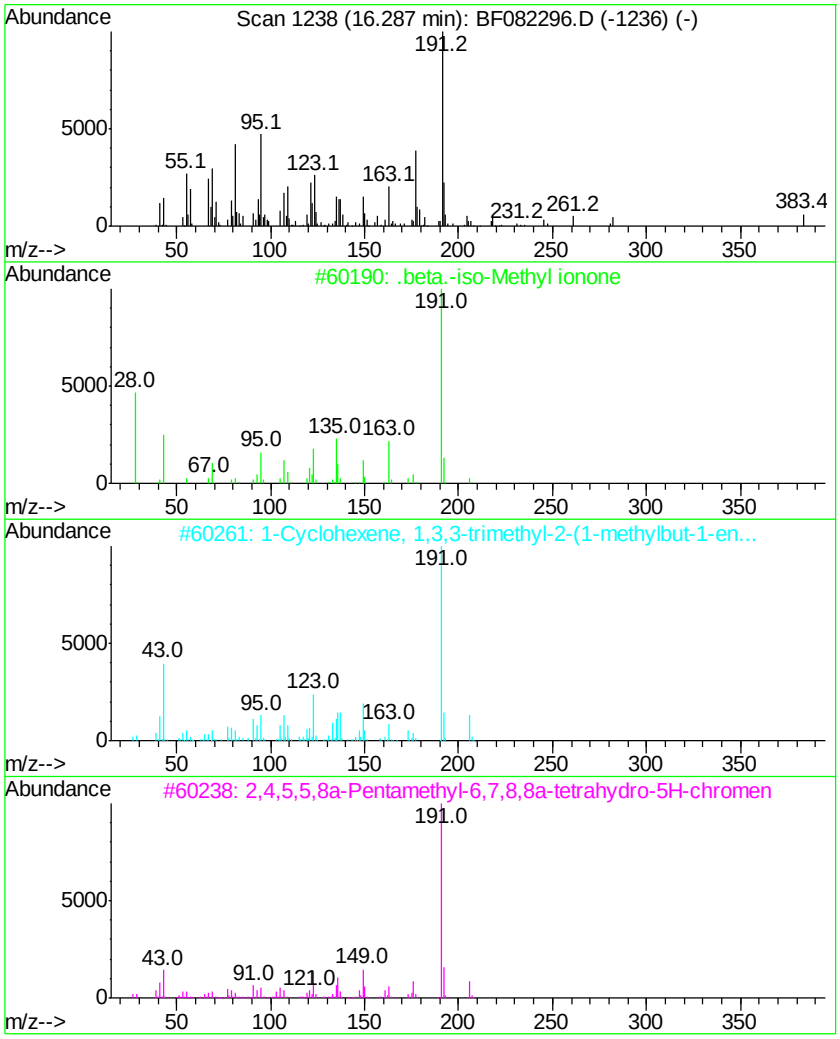
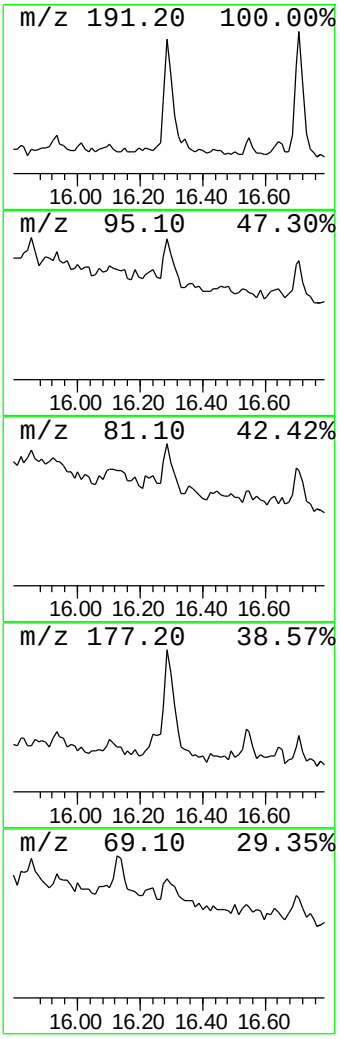
Peak Number 14 unknown16.29 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	4.60 ng	141064	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	49
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	32
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	32
4	Acetamide, N-[3-[[(2,5-dioxo-1-p...	303	C16H21N3O3	027550-64-7	27
5	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101615\
Data File : BF082296.D
Acq On : 15 Oct 2015 8:41
Operator : UM/IZ
Sample : G4016-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-8

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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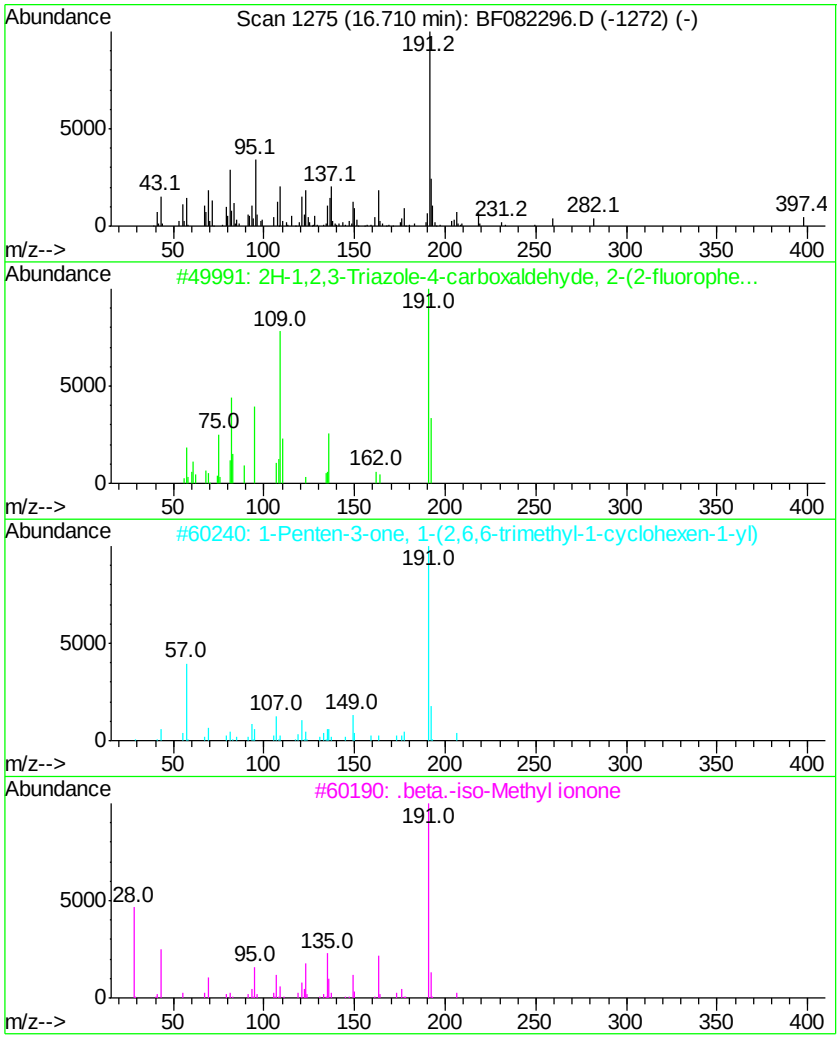
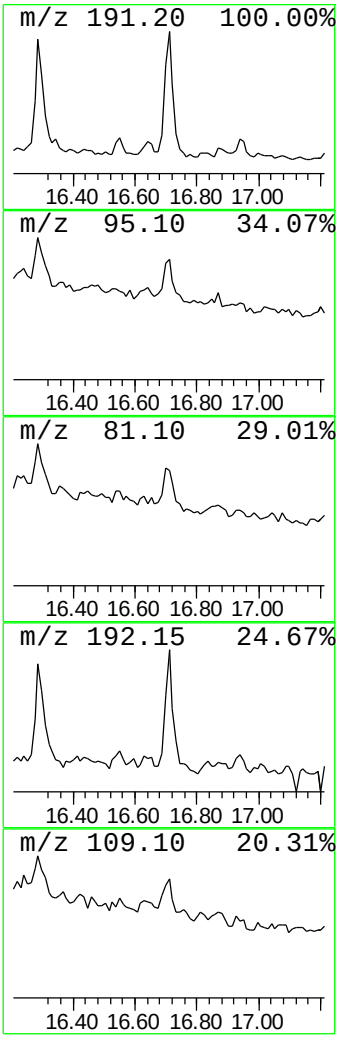
Peak Number 15 2H-1,2,3-Triazole-4-carboxa... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	6.81 ng	208865	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	50
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
5	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101615\
Data File : BF082296.D
Acq On : 15 Oct 2015 8:41
Operator : UM/IZ
Sample : G4016-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-8

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...	3.30	5.8	ng	127716	1	6.82	438086	20.0
3-Penten-2-one, 4...	4.35	265.3	ng	5810230	1	6.82	438086	20.0
2-Pentanone, 4-hy...	5.03	217.7	ng	4767750	1	6.82	438086	20.0
2-Cyclohexen-1-on...	7.15	3.0	ng	66206	1	6.82	438086	20.0
Nonadecane	10.77	3.5	ng	129374	4	11.36	741715	20.0
unknown10.98	10.98	6.5	ng	239433	4	11.36	741715	20.0
9-Eicosene, (E)-	12.40	2.8	ng	103674	4	11.36	741715	20.0
2-Propenoic acid,...	13.18	3.8	ng	114930	5	14.06	612053	20.0
unknown13.85	13.85	25.3	ng	775236	5	14.06	612053	20.0
3-Eicosene, (E)-	13.89	13.7	ng	419748	5	14.06	612053	20.0
9-Octadecenamide,...	14.92	17.7	ng	541601	6	15.61	613411	20.0
unknown16.29	16.29	4.6	ng	141064	6	15.61	613411	20.0
2H-1,2,3-Triazole...	16.71	6.8	ng	208865	6	15.61	613411	20.0