LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089609.D
Acq On : 5 Aug 2016 3:00
Operator : UM/SJ
Sample : H4348-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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-BF080416.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	4.696	266	272	274	rBV	487329	1141333	46.47%	9.075%
2	5.336	326	328	347	rBV5	165537	421257	17.15%	3.349%
3	6.970	469	471	479	rBV	139488	293863	11.97%	2.337%
4	7.085	479	481	506	rVB	562146	827395	33.69%	6.579%
5	7.439	511	512	525	rBV5	108116	221579	9.02%	1.762%
6	7.679	530	533	552	rVB	1062814	1482946	60.38%	11.791%
7	8.353	589	592	615	rBV	677702	1215520	49.49%	9.665%
8	8.696	618	622	635	rVB	106670	165964	6.76%	1.320%
9	9.462	687	689	702	rBV	176205	320160	13.04%	2.546%
10	11.256	842	846	867	rBV	1544894	2455904	100.00%	19.527%
11	11.942	904	906	912	rBV	50971	77287	3.15%	0.615%
12	12.285	934	936	939	rBV	246099	380091	15.48%	3.022%
13	12.399	943	946	949	rVB	43120	47170	1.92%	0.375%
14	13.005	996	999	1003	rBV	46093	61547	2.51%	0.489%
15	13.154	1008	1012	1014	rBV	43162	65559	2.67%	0.521%
16	13.508	1037	1043	1047	rBV	15225	41579	1.69%	0.331%
17	13.577	1047	1049	1054	rBV	420229	581659	23.68%	4.625%
18	13.920	1076	1079	1087	rVB2	58389	96090	3.91%	0.764%
19	14.651	1140	1143	1144	rBV	21652	24947	1.02%	0.198%
20	14.685	1144	1146	1162	rVB	271204	399053	16.25%	3.173%
21	17.051	1350	1353	1356	rBV	1240318	1588262	64.67%	12.628%
22	18.320	1461	1464	1468	rBV	45298	118649	4.83%	0.943%
23	18.377	1468	1469	1475	rVB	226221	308846	12.58%	2.456%
24	20.046	1612	1615	1624	rBV	137594	240194	9.78%	1.910%

Sum of corrected areas: 12576854

LSC Report - Integrated Chromatogram

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Misc :
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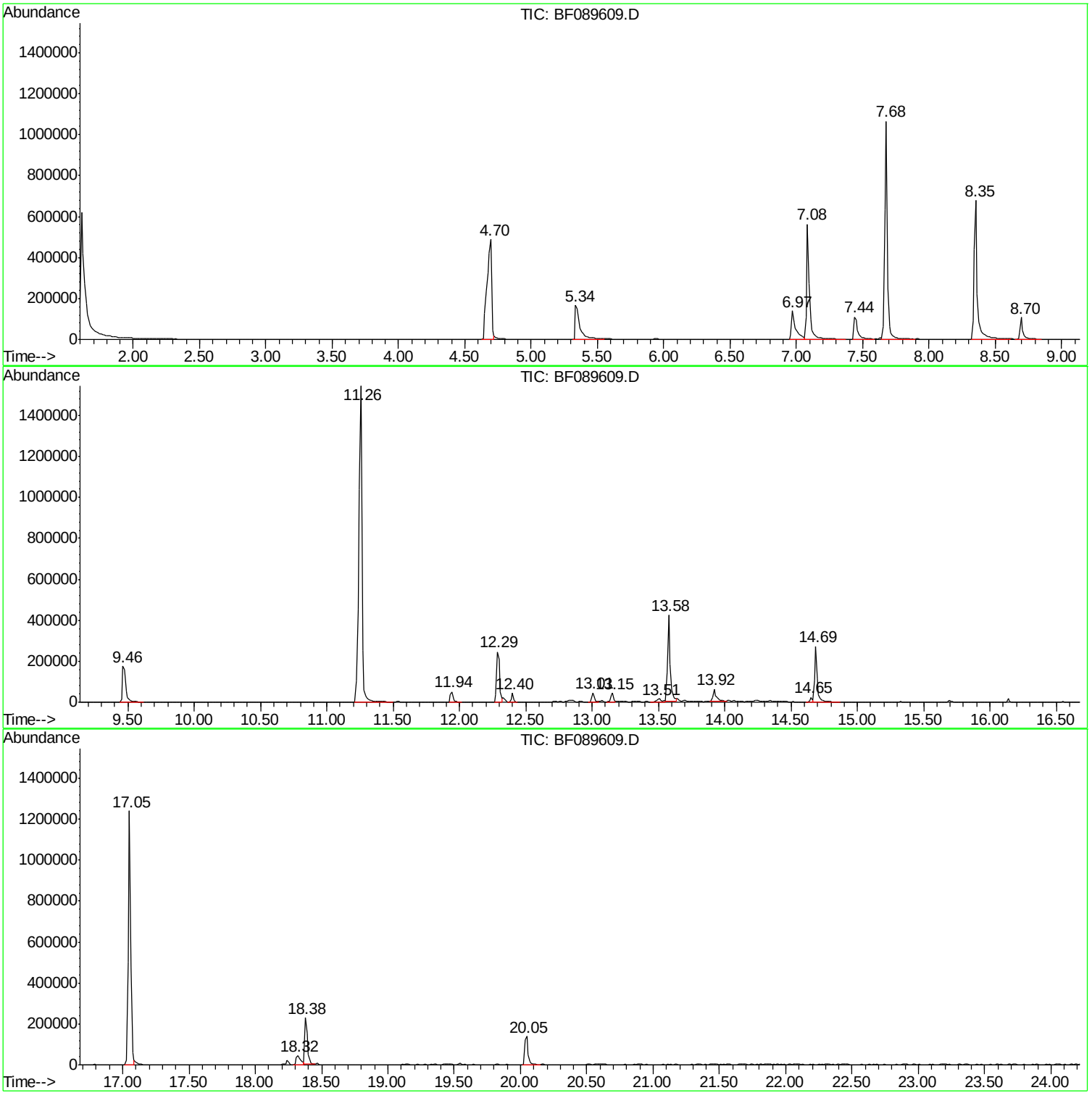
Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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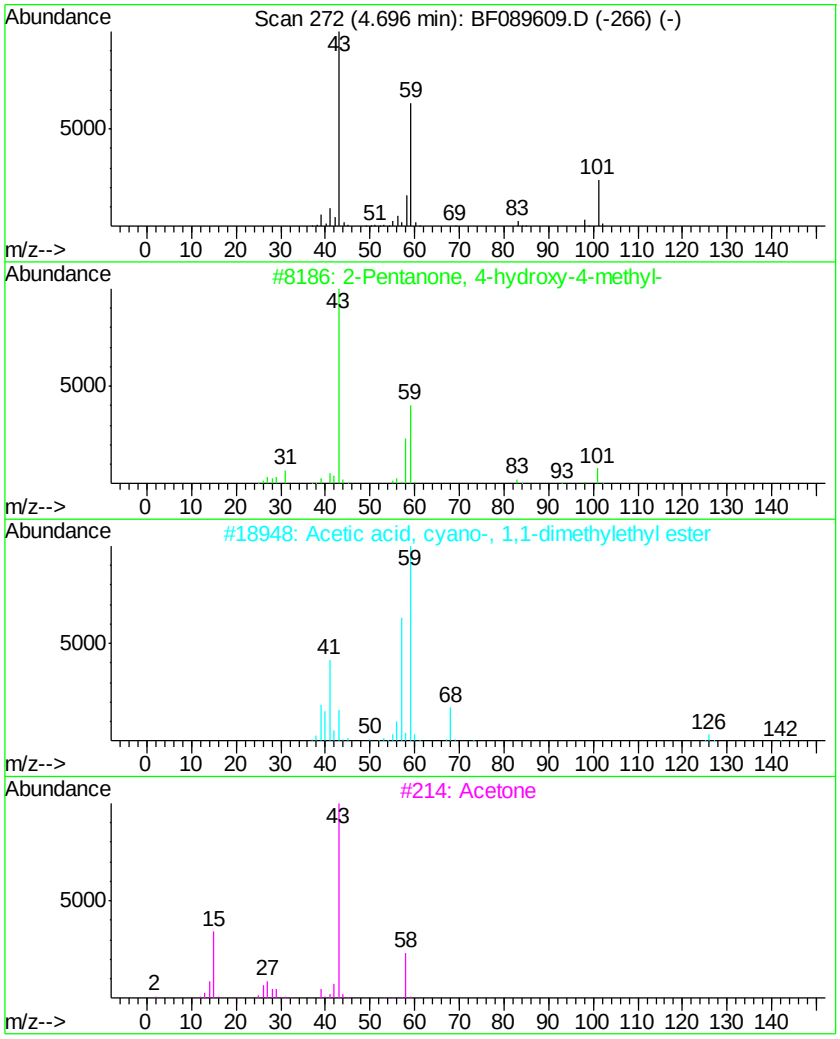
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

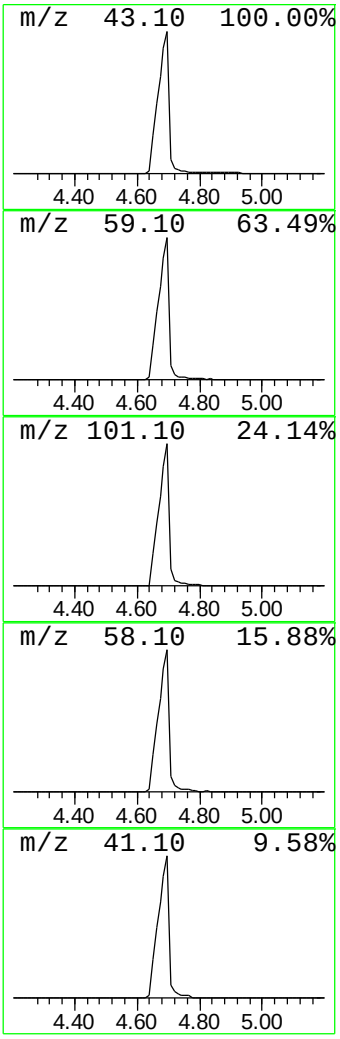
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	103.02 ng	1141330	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
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TIC Library : C:\Database\NIST11.L
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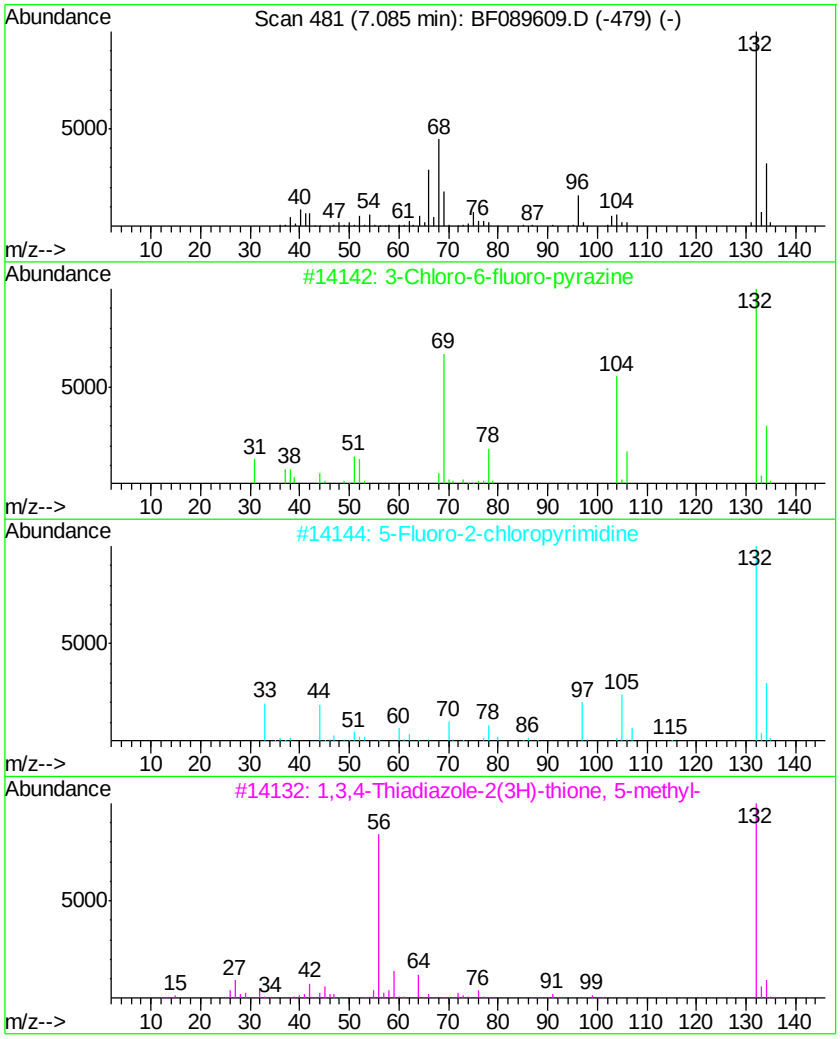
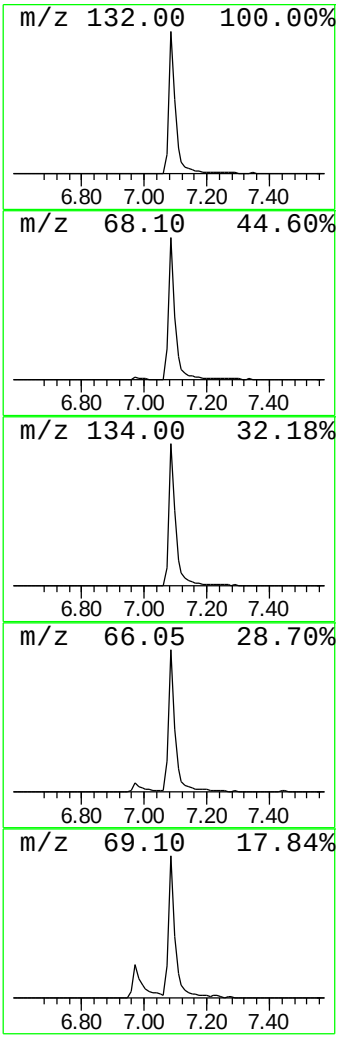
****

Peak Number 2 unknown7.08 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	74.68 ng	827395	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





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Sample : H4348-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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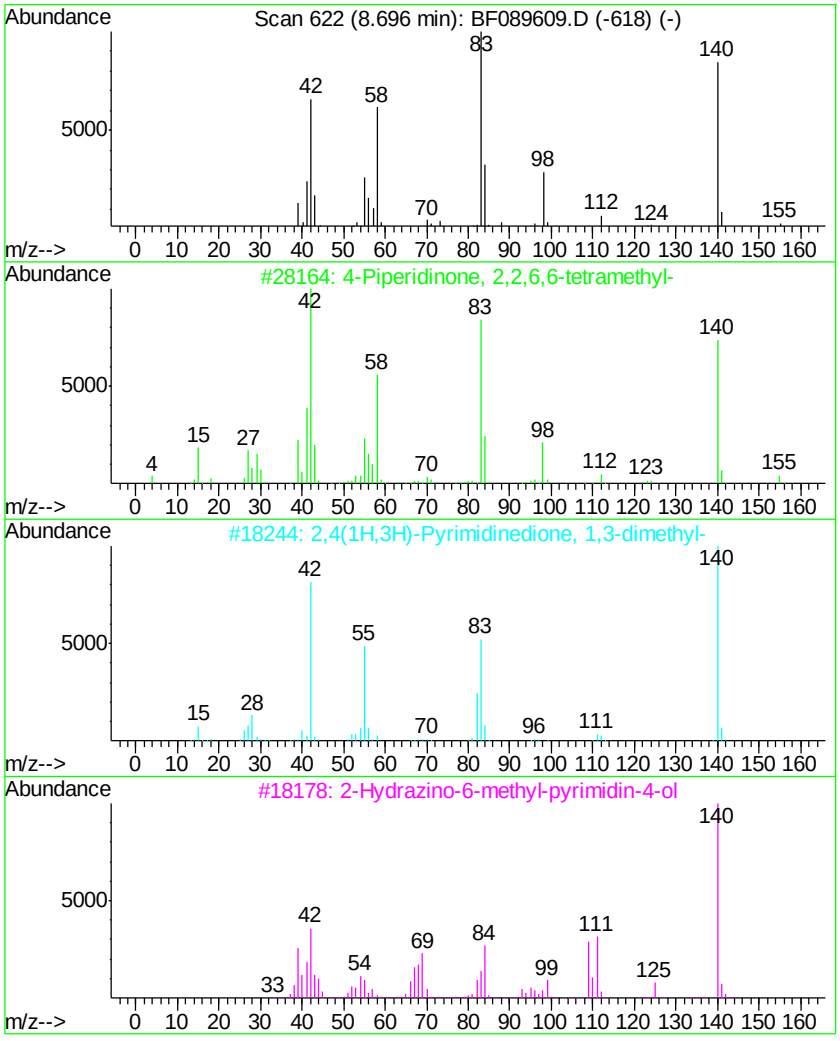
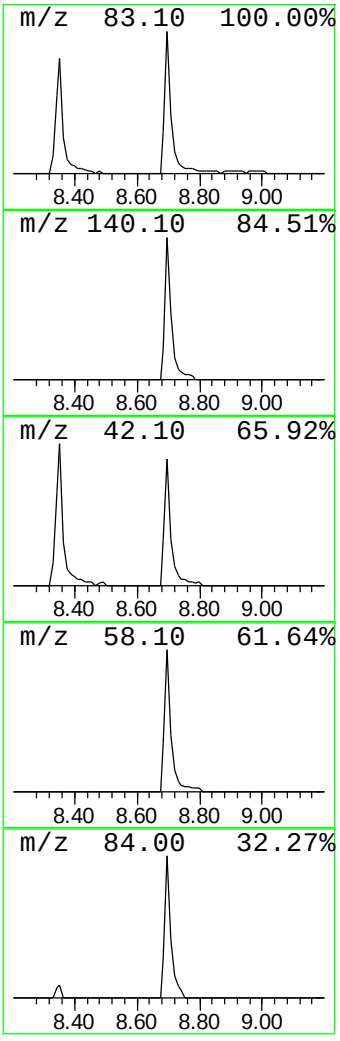
Peak Number 4 4-Piperidinone, 2,2,6,6-tet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	10.37 ng	165964	Naphthalene-d8	9.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Piperidinone, 2,2,6,6-tetramet...	155	C9H17NO	000826-36-8	91
2	2,4(1H,3H)-Pyrimidinedione, 1,3-...	140	C6H8N2O2	000874-14-6	35
3	2-Hydrazino-6-methyl-pyrimidin-4-ol	140	C5H8N4O	037893-08-6	32
4	1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	32
5	1H-Pyrazole, 4,5-dihydro-5,5-dim...	98	C5H10N2	004320-85-8	32





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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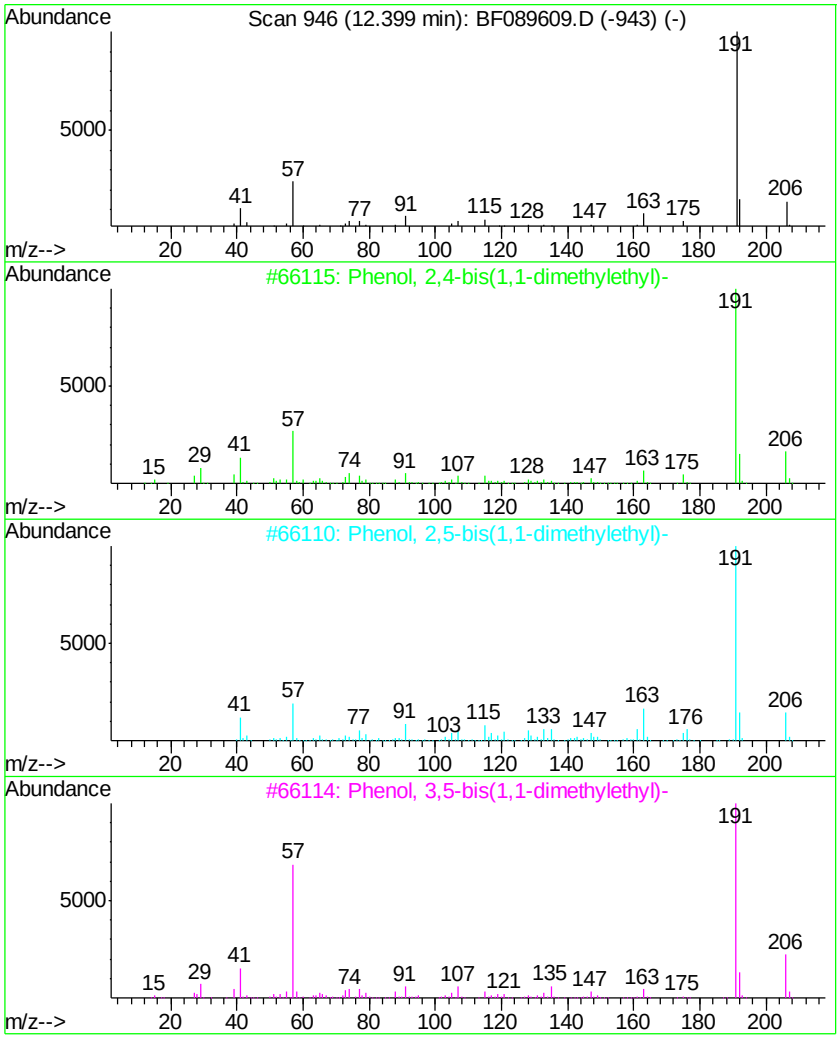
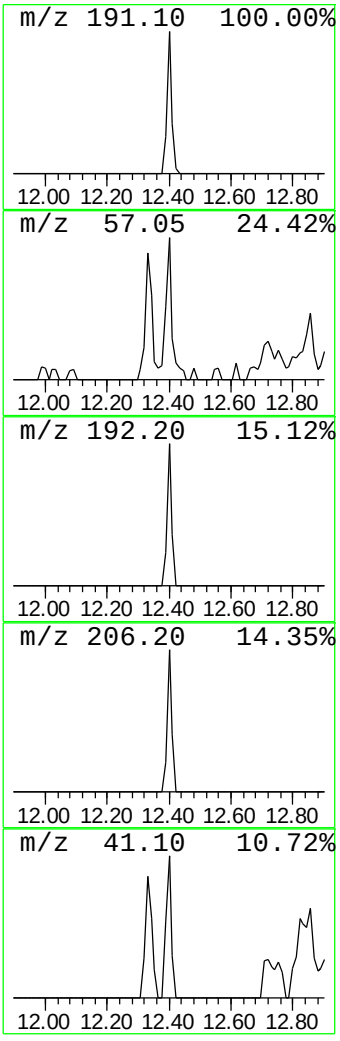
Peak Number 5 Phenol, 2,4-bis(1,1-dimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	2.48 ng	47170	Acenaphthene-d10	12.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	97
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	91
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	87
4	Pentanoic acid, 5-hydroxy-, 2,4-...	306	C19H30O3	166273-38-7	83
5	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
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Operator : UM/SJ
Sample : H4348-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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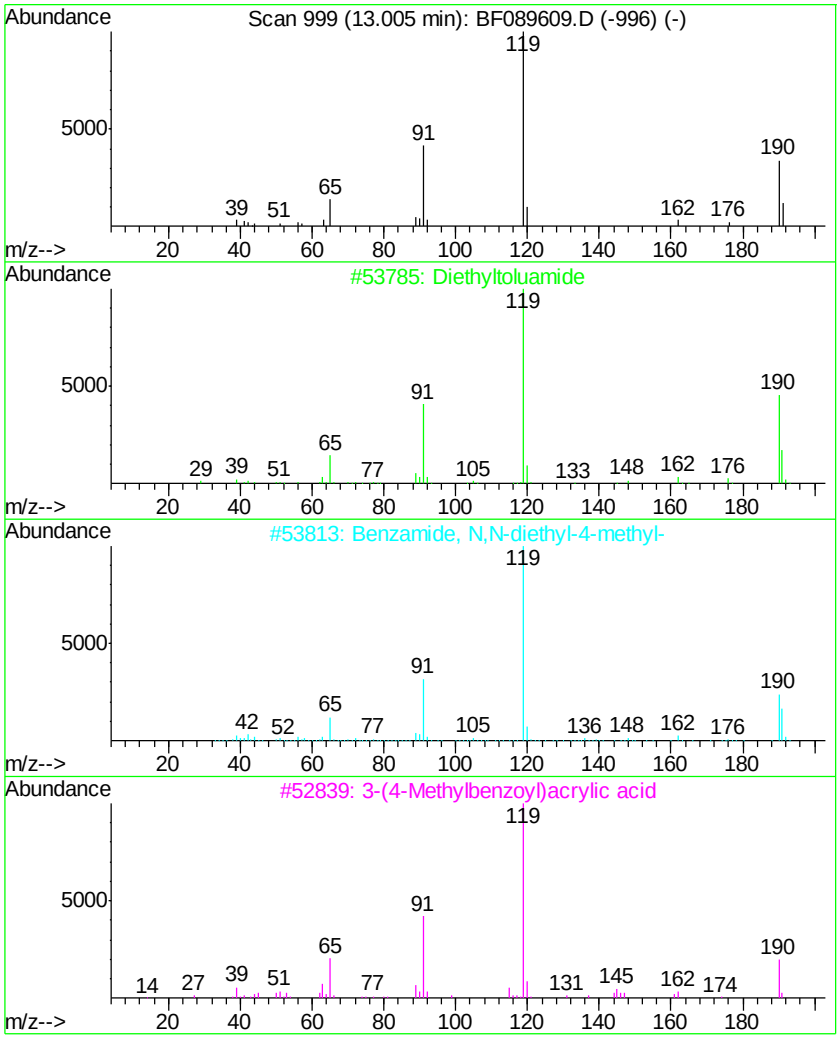
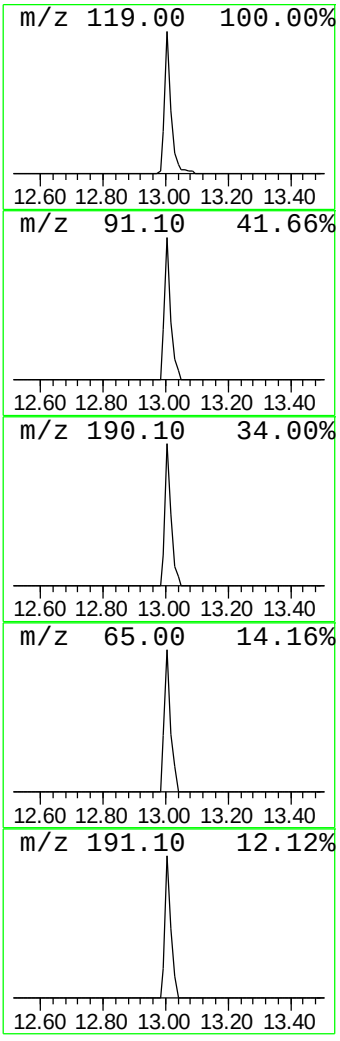
Peak Number 6 Diethyltoluamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	3.24 ng	61547	Acenaphthene-d10	12.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	86
3	3-(4-Methylbenzoyl)acrylic acid	190	C11H10O3	020972-36-5	78
4	l-Valine, N-(p-toluoyl)-, methyl...	249	C14H19NO3	1000299-64-7	78
5	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	72





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Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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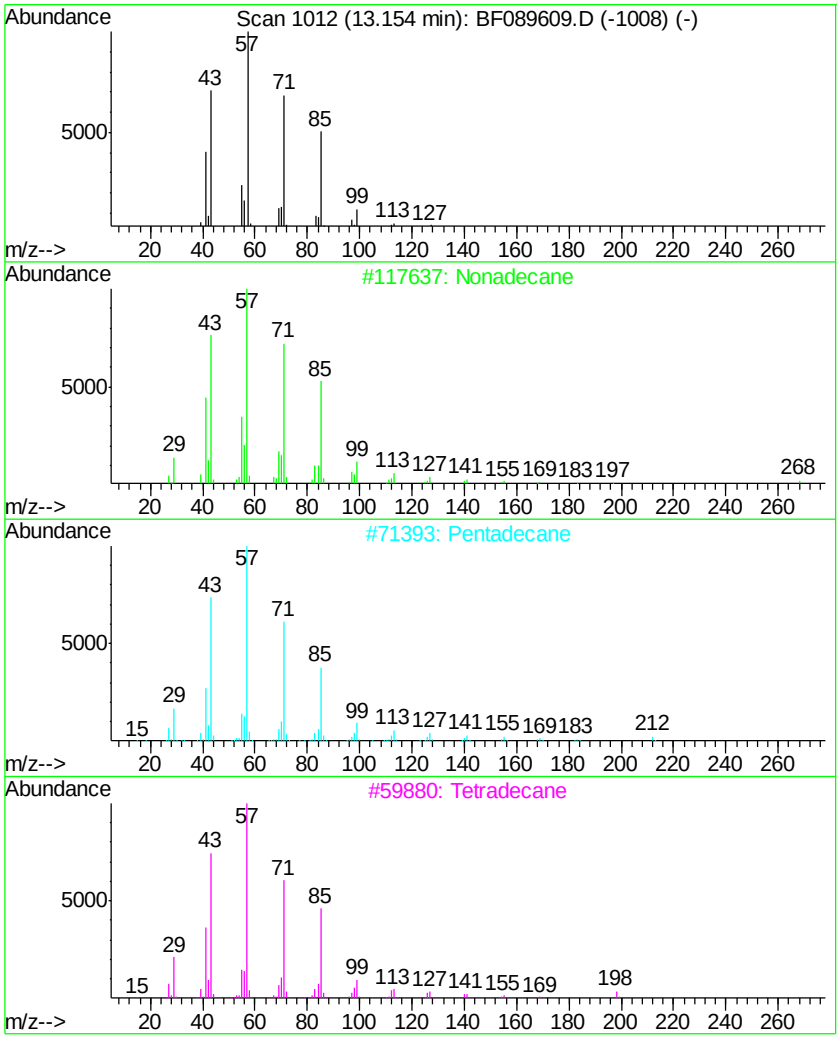
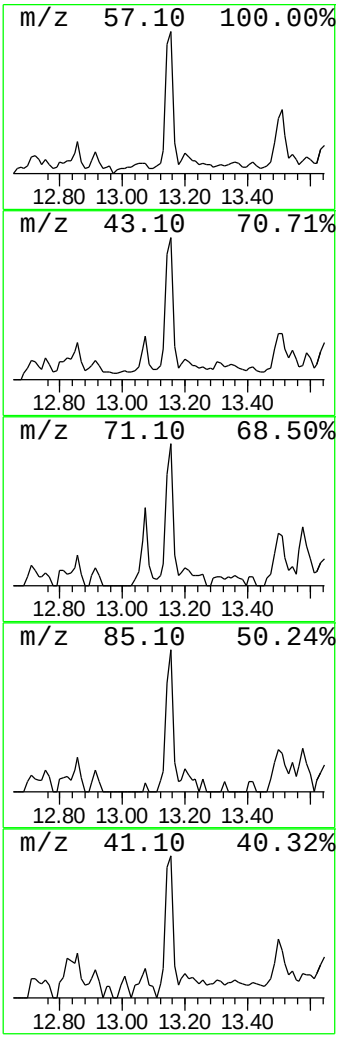
Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	3.45 ng	65559	Acenaphthene-d10	12.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Pentadecane	212	C15H32	000629-62-9	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
5	Hexadecane	226	C16H34	000544-76-3	78





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TIC Library : C:\Database\NIST11.L
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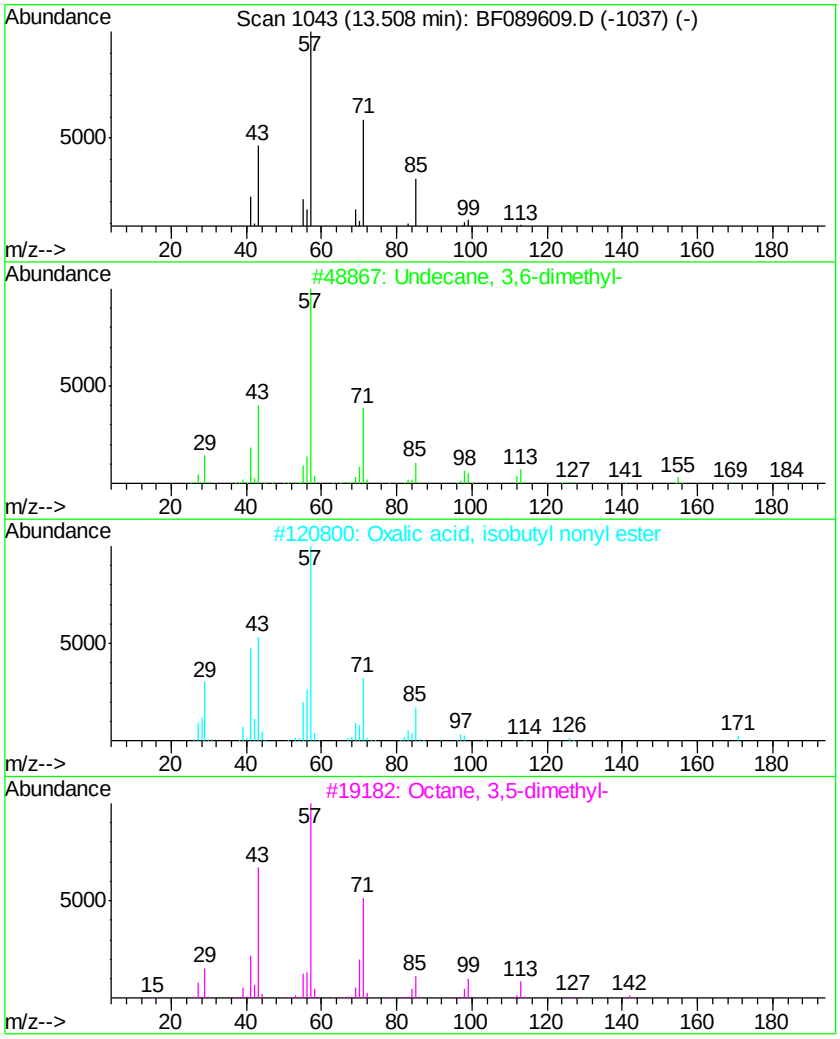
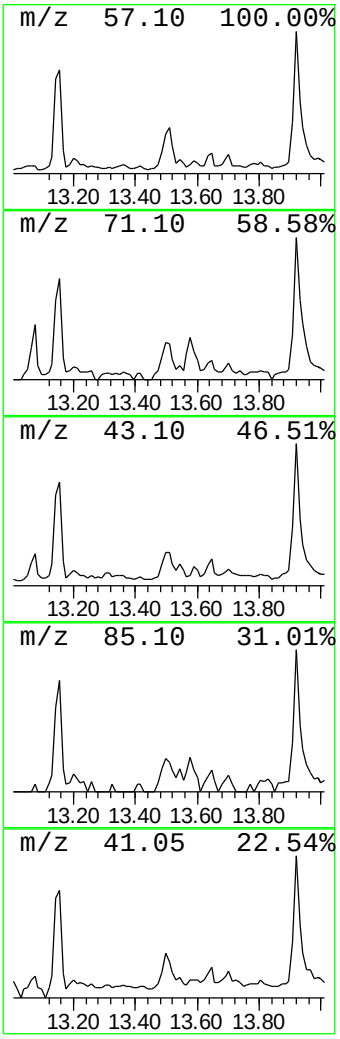
Peak Number 8 Undecane, 3,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	2.08 ng	41579	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
2	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	56
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
4	Dotriacontane	451	C32H66	000544-85-4	53
5	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	50





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-2

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TIC Library : C:\Database\NIST11.L
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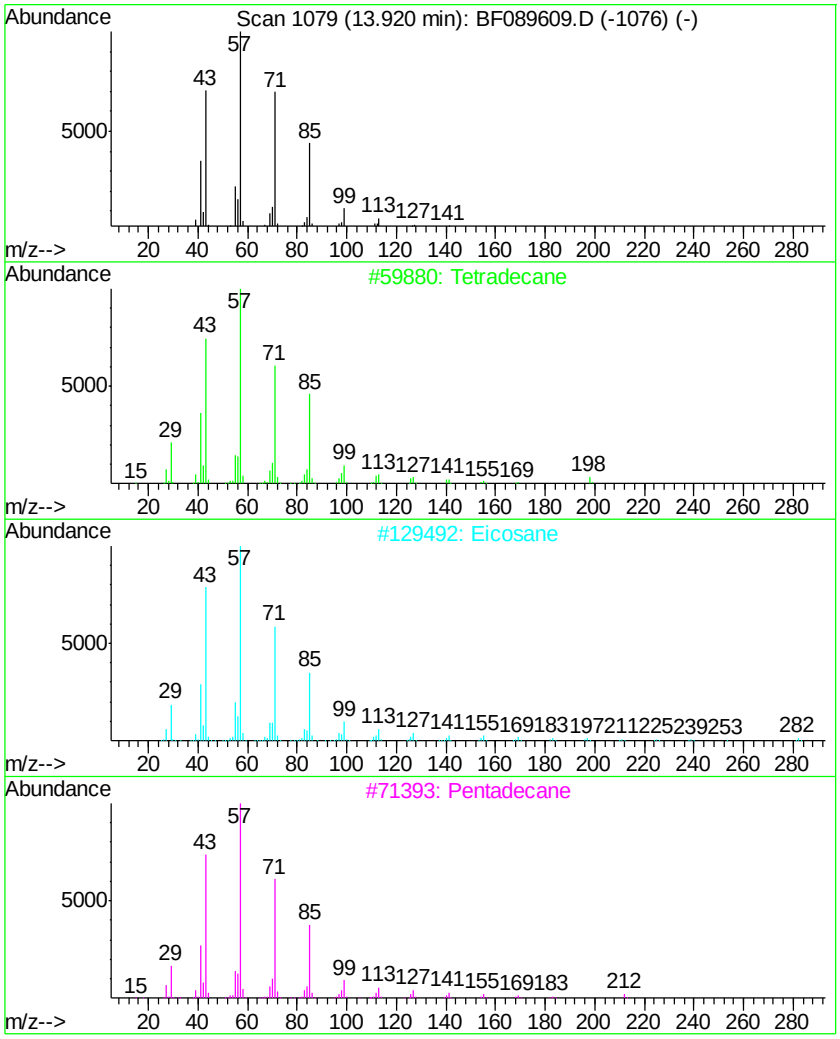
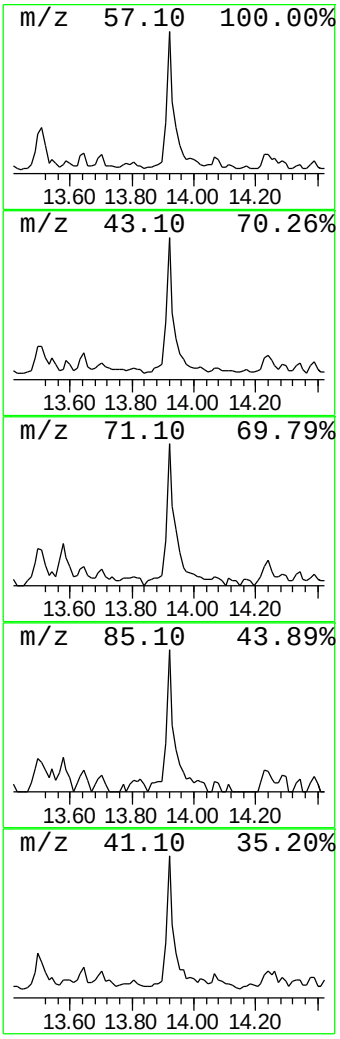
Peak Number 9 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.82 ng	96090	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Nonadecane	268	C19H40	000629-92-5	78
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	78





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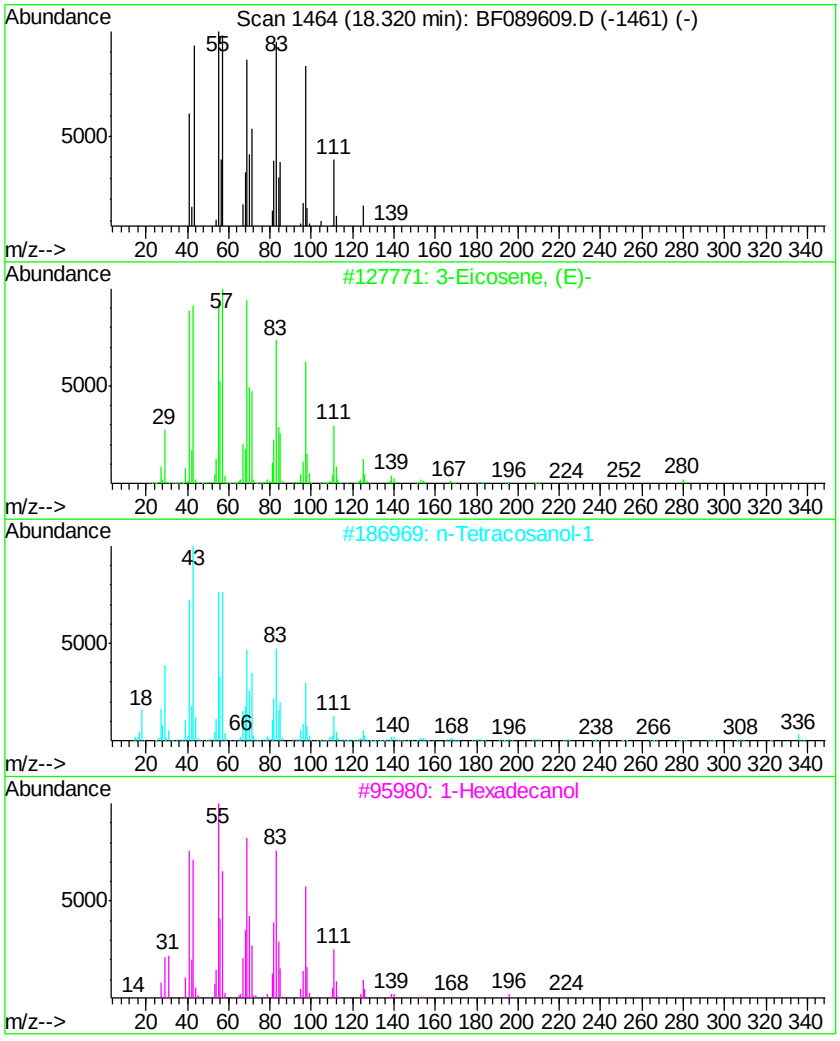
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

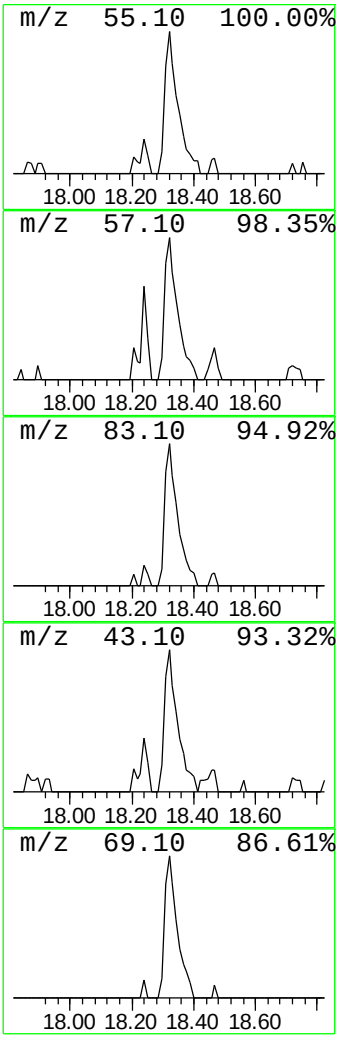
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	7.68 ng	118649	Chrysene-d12	18.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	86
5	1-Docosene	308	C22H44	001599-67-3	81





Tentatively Identified Compound (LSC) summary

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Data File : BF089609.D
Acq On : 5 Aug 2016 3:00
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	103.0	ng	1141330	1	7.44	221579	20.0
unknown7.08	7.08	74.7	ng	827395	1	7.44	221579	20.0
4-Piperidinone, 2...	8.70	10.4	ng	165964	2	9.46	320160	20.0
Phenol, 2,4-bis(1...	12.40	2.5	ng	47170	3	12.29	380091	20.0
Diethyltoluamide	13.01	3.2	ng	61547	3	12.29	380091	20.0
Nonadecane	13.15	3.5	ng	65559	3	12.29	380091	20.0
Undecane, 3,6-dim...	13.51	2.1	ng	41579	4	14.69	399053	20.0
Tetradecane	13.92	4.8	ng	96090	4	14.69	399053	20.0
3-Eicosene, (E)-	18.32	7.7	ng	118649	5	18.38	308846	20.0