LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096082.D
Acq On : 21 Jun 2017 13:55
Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

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-BF060517.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	1.552	9	11	35	rVB	570808	1260584	25.72%	4.617%
2	2.369	146	150	170	rBV2	26599	65796	1.34%	0.241%
3	3.446	329	333	352	rBV2	61399	206592	4.21%	0.757%
4	4.504	509	513	535	rBV	78374	249677	5.09%	0.914%
5	5.204	628	632	666	rBV	740158	1904340	38.85%	6.974%
6	6.875	912	916	926	rBV	643005	1460489	29.79%	5.349%
7	6.951	926	929	960	rVB	1212666	2301222	46.94%	8.428%
8	7.292	982	987	1000	rVB	294194	422783	8.62%	1.548%
9	7.528	1022	1027	1051	rVB	1049930	1450352	29.59%	5.312%
10	8.210	1138	1143	1169	rBV	693125	1141181	23.28%	4.179%
11	9.322	1327	1332	1348	rBV	400336	597813	12.20%	2.189%
12	11.098	1628	1634	1645	rBV	1602130	2304273	47.01%	8.439%
13	12.139	1806	1811	1819	rBV2	459719	643385	13.12%	2.356%
14	12.710	1900	1908	1919	rBV	67645	120163	2.45%	0.440%
15	13.439	2027	2032	2051	rBV	896895	1309901	26.72%	4.797%
16	14.221	2157	2165	2174	rBV	59740	95672	1.95%	0.350%
17	14.533	2213	2218	2233	rBV	471570	667039	13.61%	2.443%
18	15.598	2383	2399	2422	rBV	921668	2243055	45.76%	8.215%
19	16.145	2486	2492	2500	rBV5	35731	57537	1.17%	0.211%
20	16.539	2552	2559	2561	rBV	180652	293485	5.99%	1.075%
21	16.562	2561	2563	2573	rVB2	124278	177893	3.63%	0.651%
22	16.721	2574	2590	2593	rBV	1978241	4902018	100.00%	17.952%
23	16.927	2619	2625	2628	rBV	1951976	2443736	49.85%	8.950%
24	18.268	2848	2853	2862	rBV	454545	587167	11.98%	2.150%
25	19.944	3134	3138	3148	rBV2	247766	399568	8.15%	1.463%

Sum of corrected areas: 27305721

LSC Report - Integrated Chromatogram

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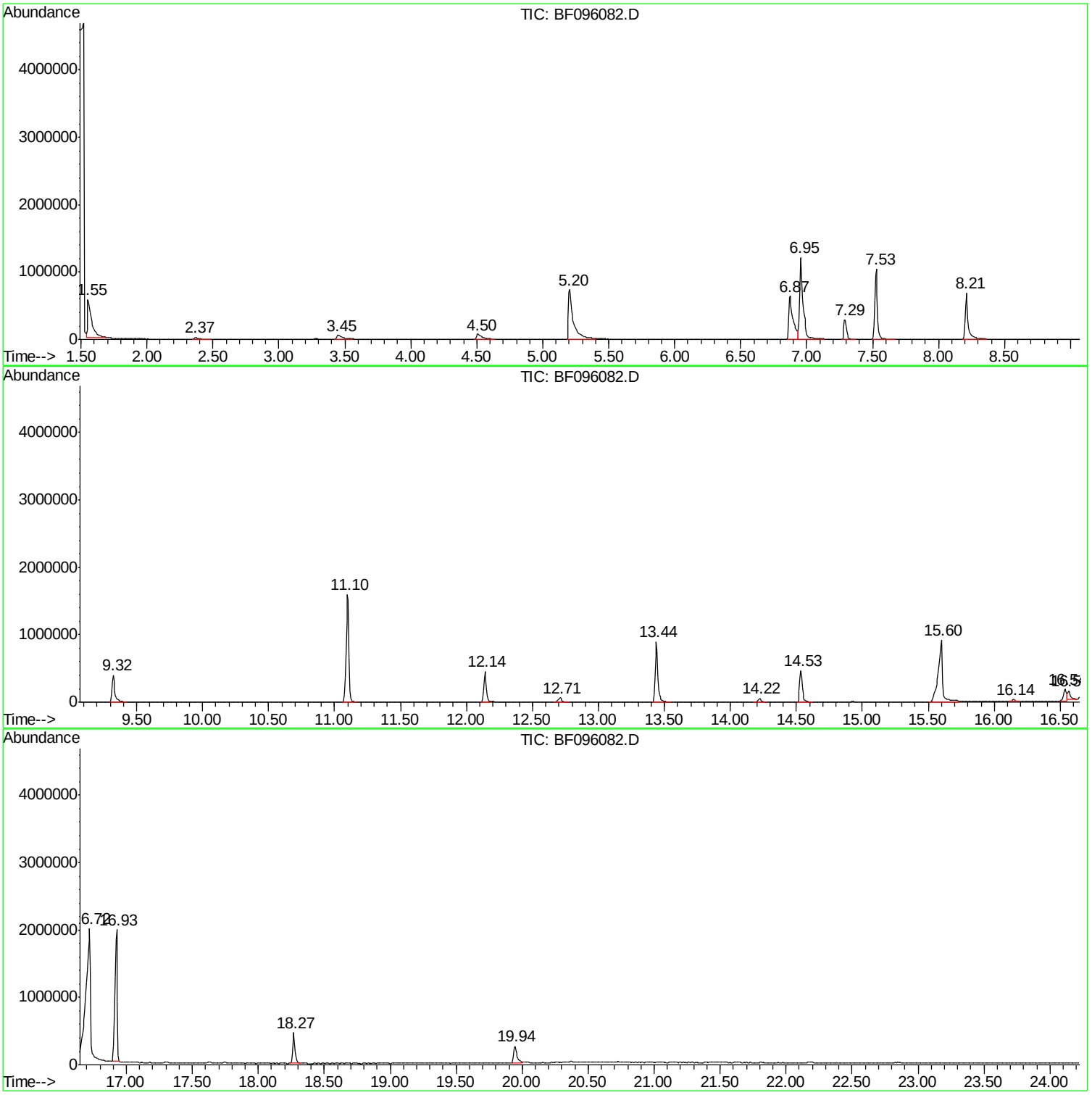
Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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Operator : SJ/MA
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Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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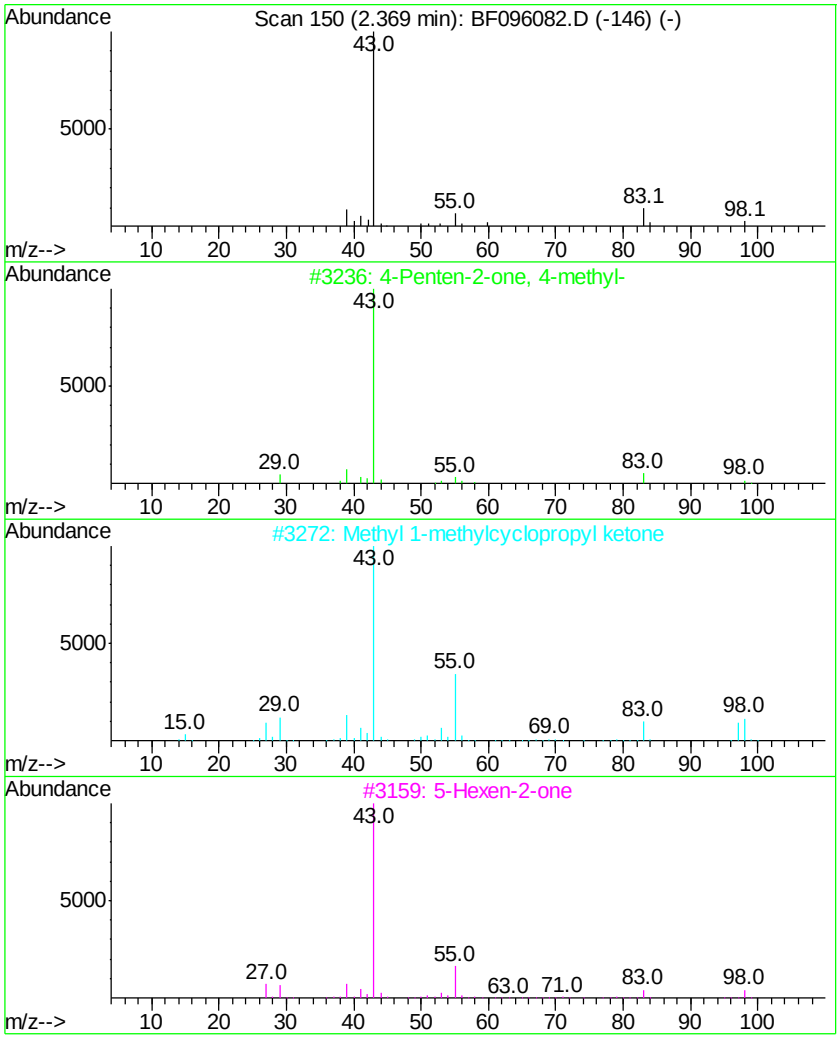
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

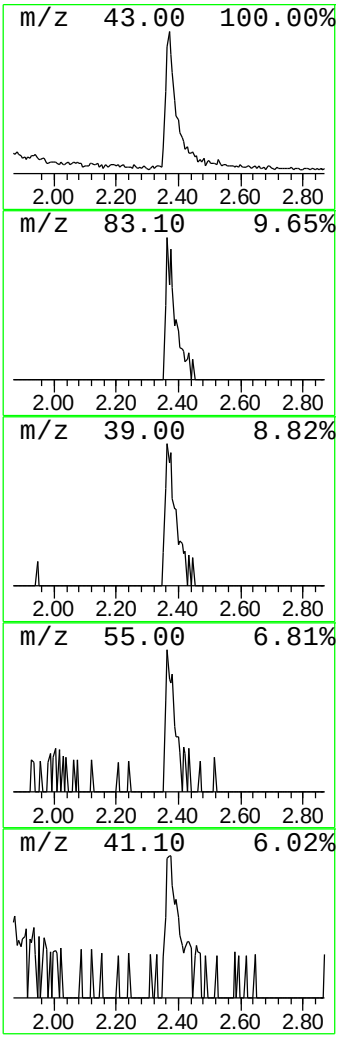
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	3.11 ng	65796	1,4-Dichlorobenzene-d4	7.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	47
3	5-Hexen-2-one	98	C6H10O	000109-49-9	40
4	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	5





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Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

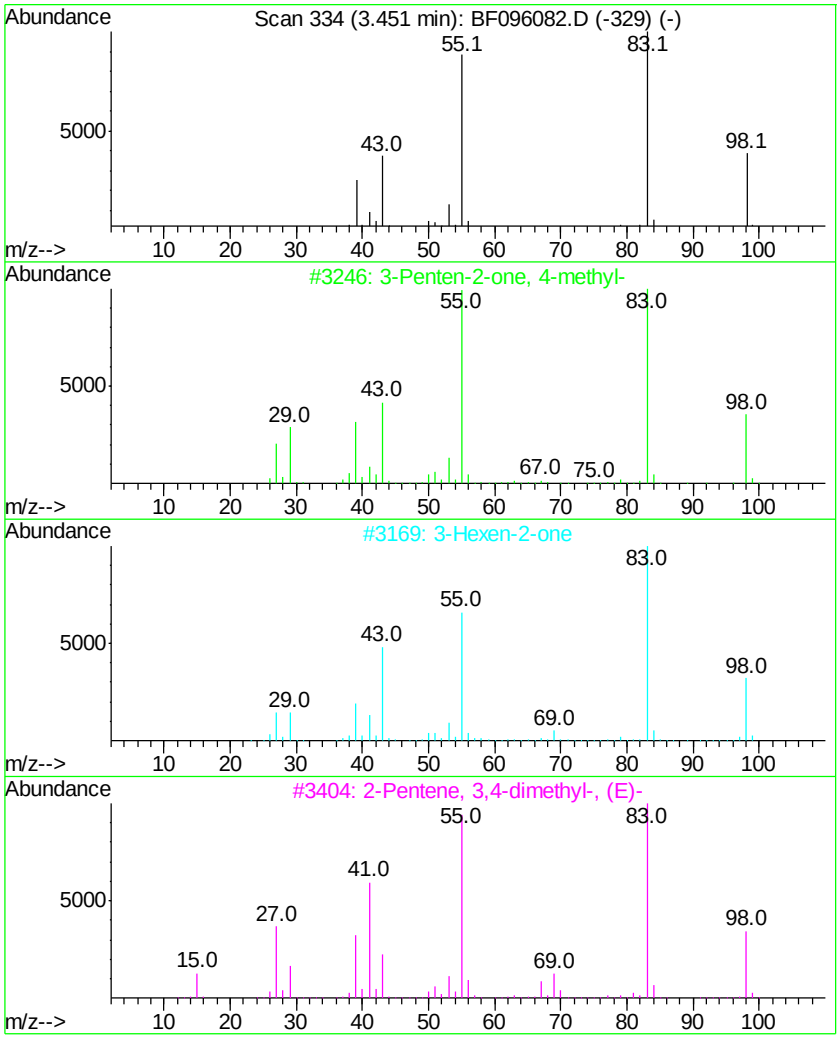
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

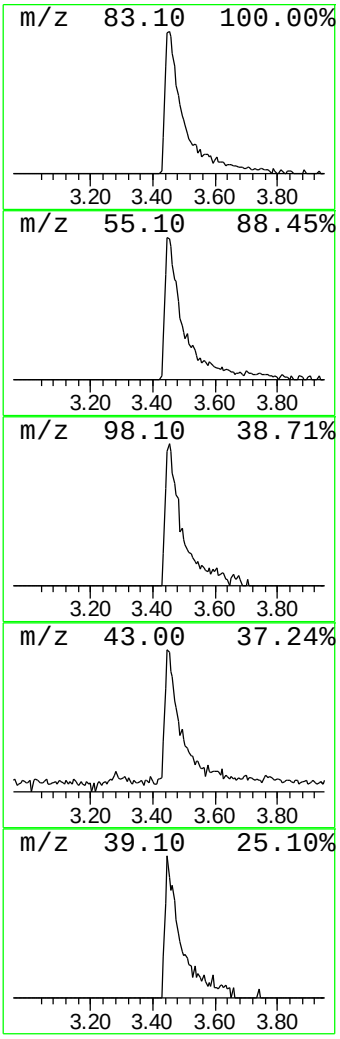
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.45	9.77 ng	206592	1,4-Dichlorobenzene-d4	7.29

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	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096082.D
Acq On : 21 Jun 2017 13:55
Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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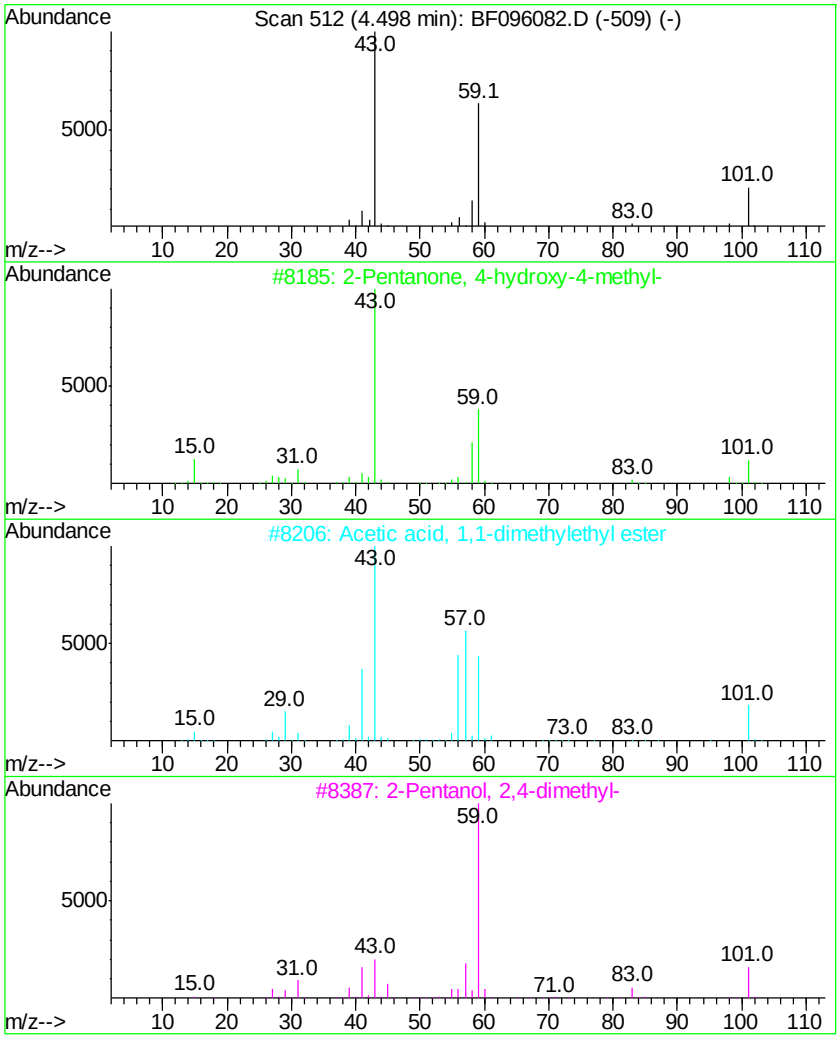
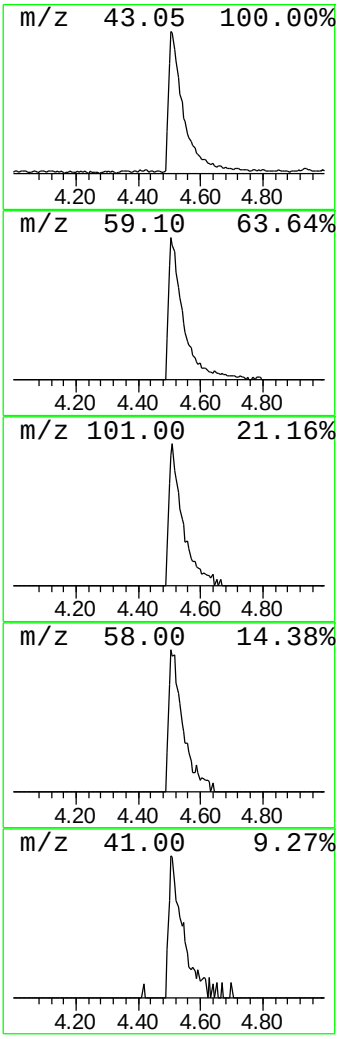
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	11.81 ng	249677	1,4-Dichlorobenzene-d4	7.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
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Acq On : 21 Jun 2017 13:55
Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

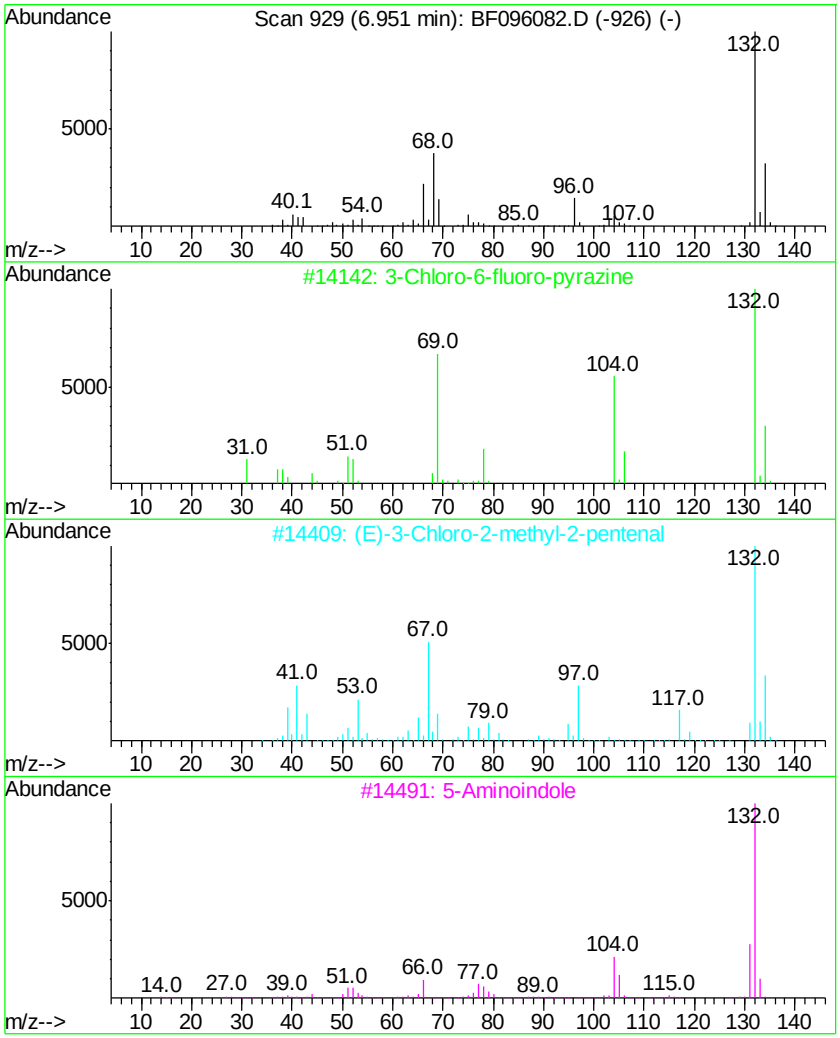
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

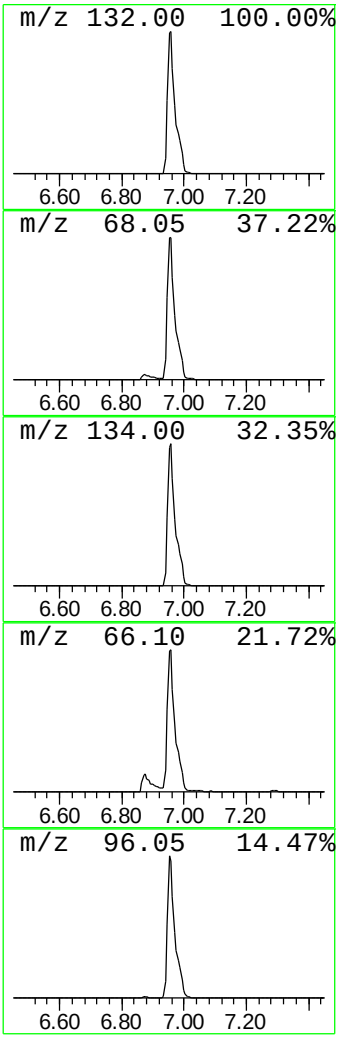
****

Peak Number 5 unknown6.95 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	108.86 ng	2301220	1,4-Dichlorobenzene-d4	7.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Operator : SJ/MA
Sample : I3759-03
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

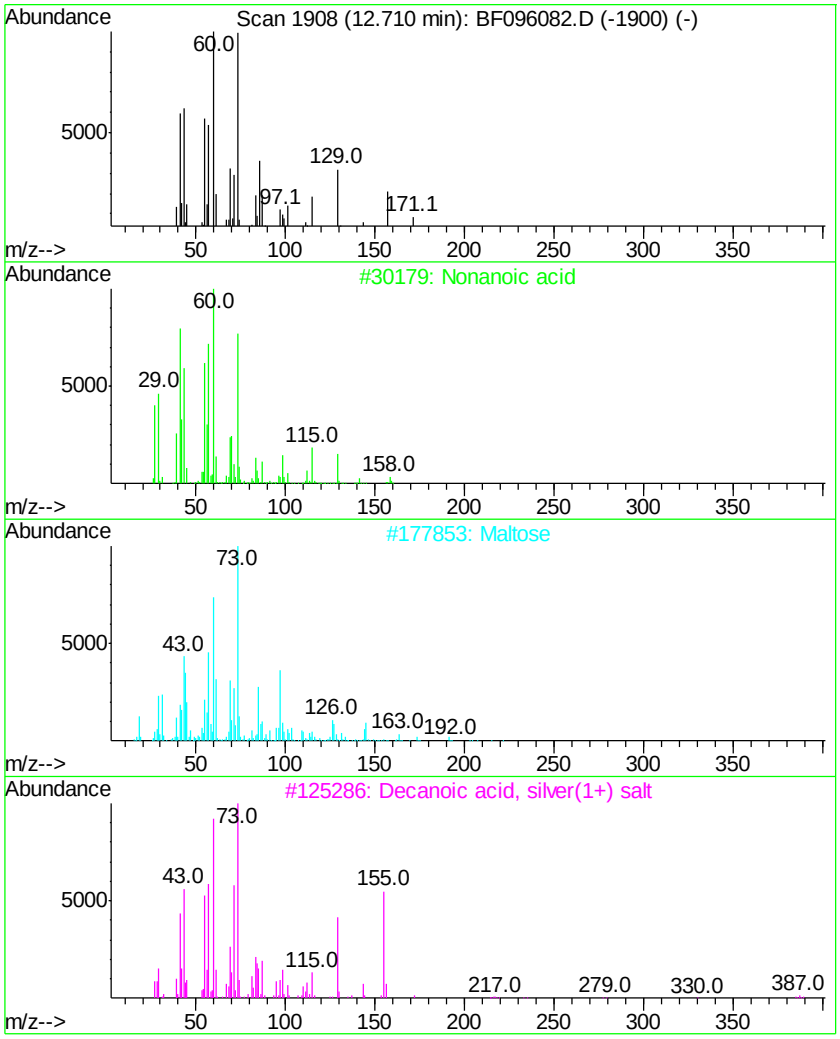
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

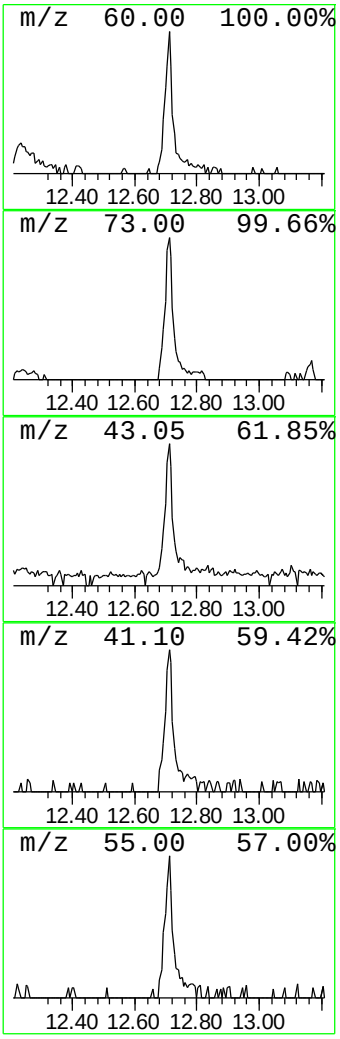
****

Peak Number 7 Nonanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.74 ng	120163	Acenaphthene-d10	12.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	50
2	Maltose	342	C12H22O11	000069-79-4	47
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	45
4	.alpha.-D-Glucose	180	C6H12O6	000492-62-6	38
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38





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Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

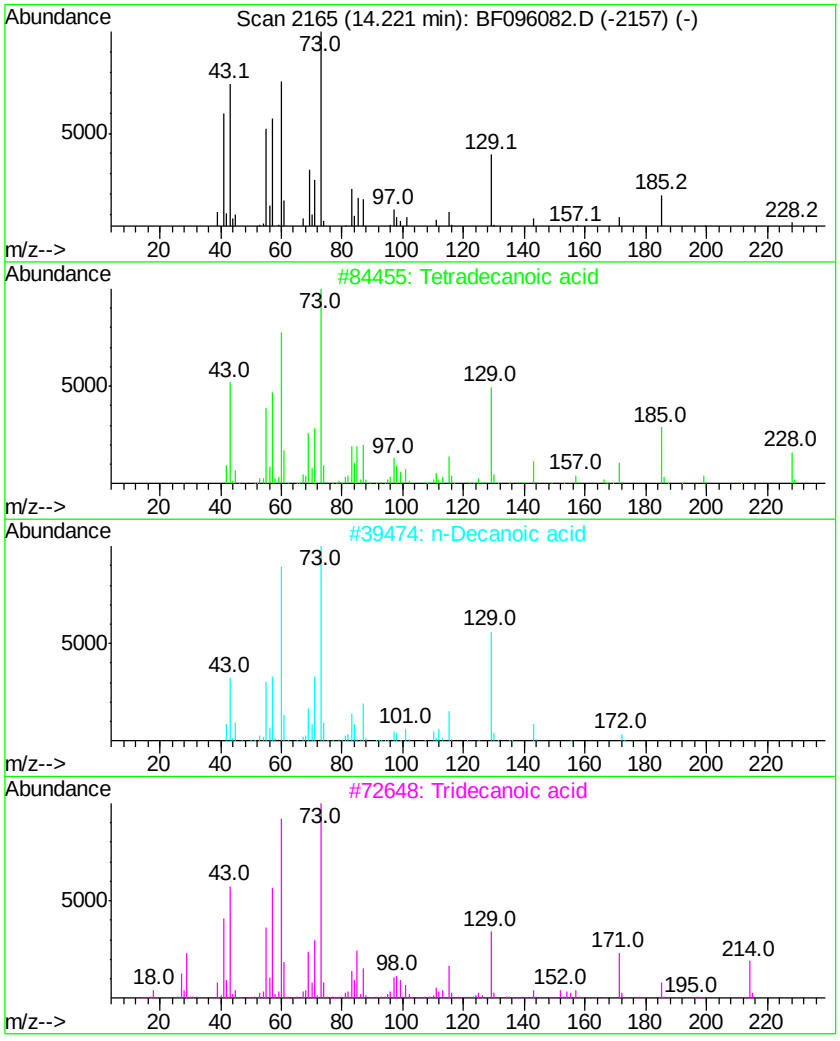
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

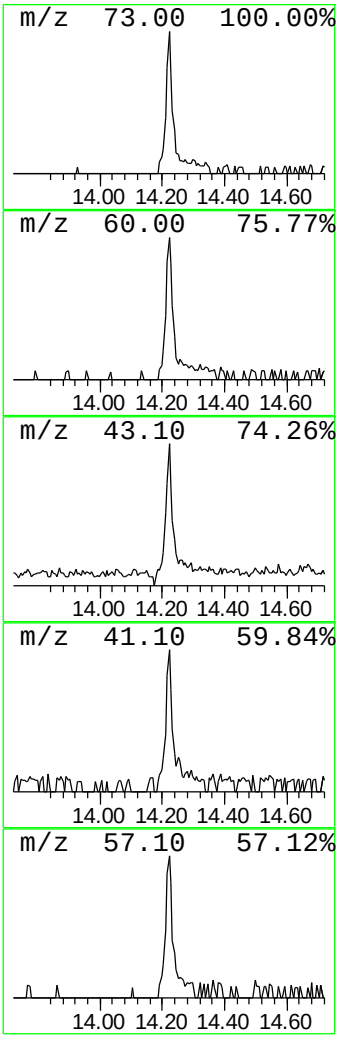
****

Peak Number 8 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.87 ng	95672	Phenanthrene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Heptanoic acid	130	C7H14O2	000111-14-8	38





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Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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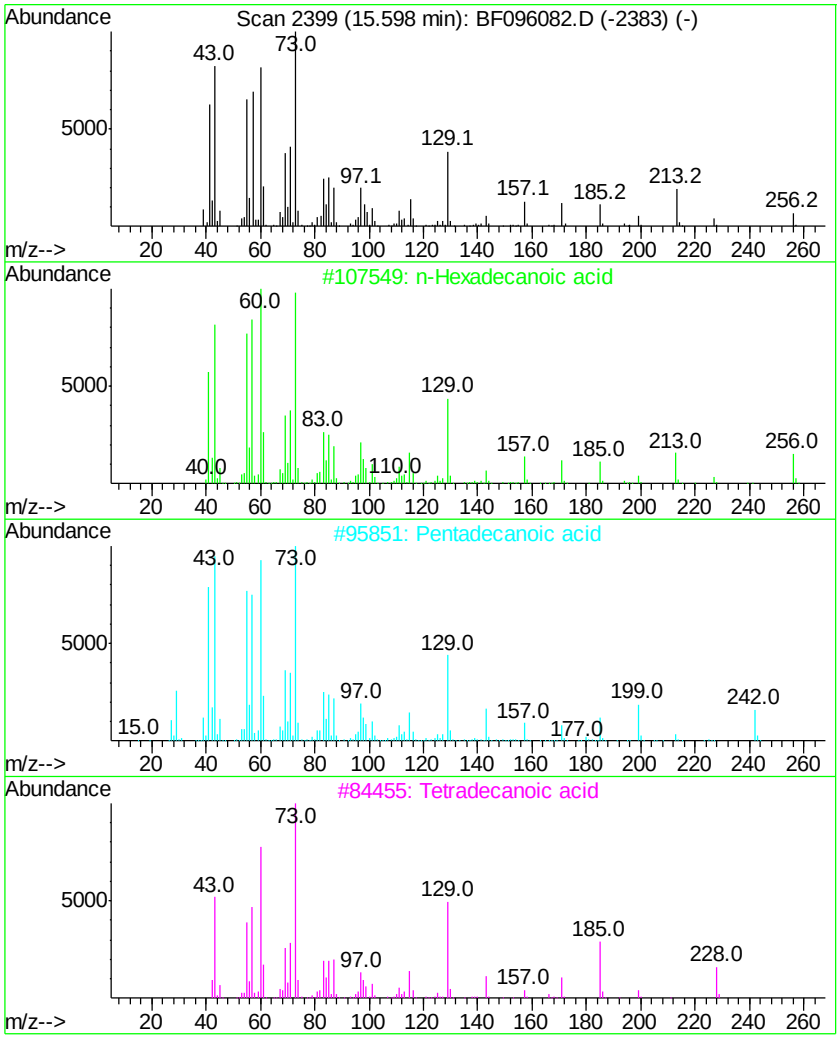
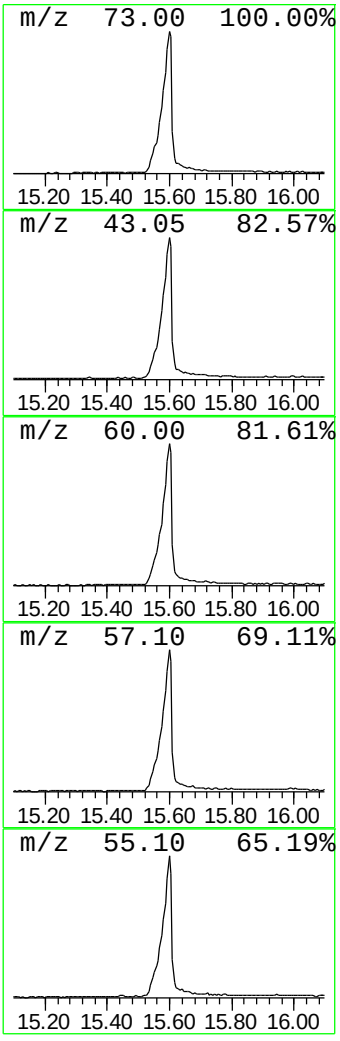
Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	67.25 ng	2243060	Phenanthrene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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

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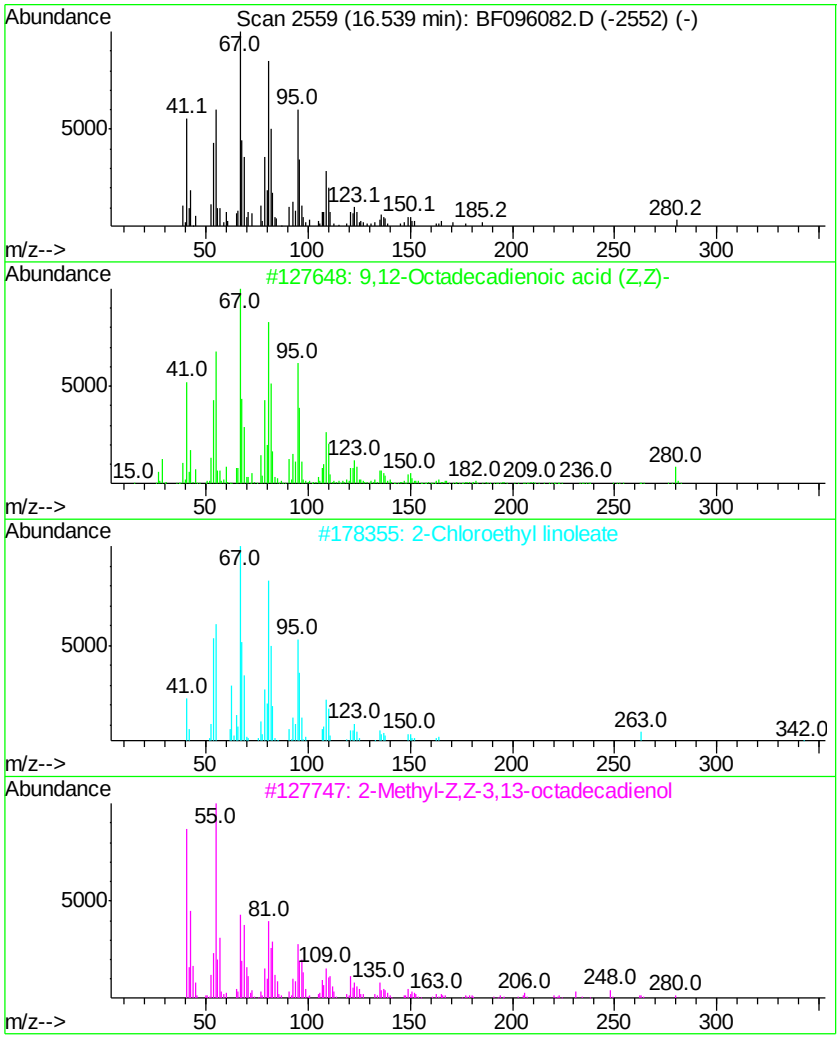
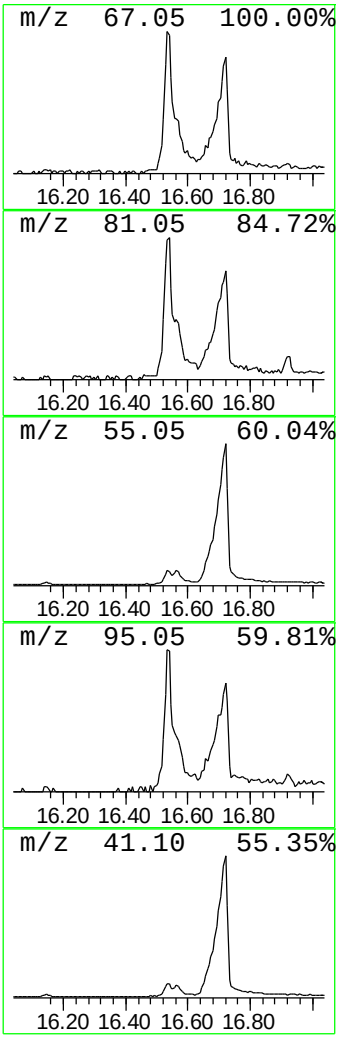
Peak Number 10 9,12-Octadecadienoic acid (... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	10.00 ng	293485	Chrysene-d12	18.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
3	2-Methyl-Z,Z-3,13-octadecadienol	280	C19H36O	1000130-90-5	90
4	8-Hexadecyne	222	C16H30	019781-86-3	87
5	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

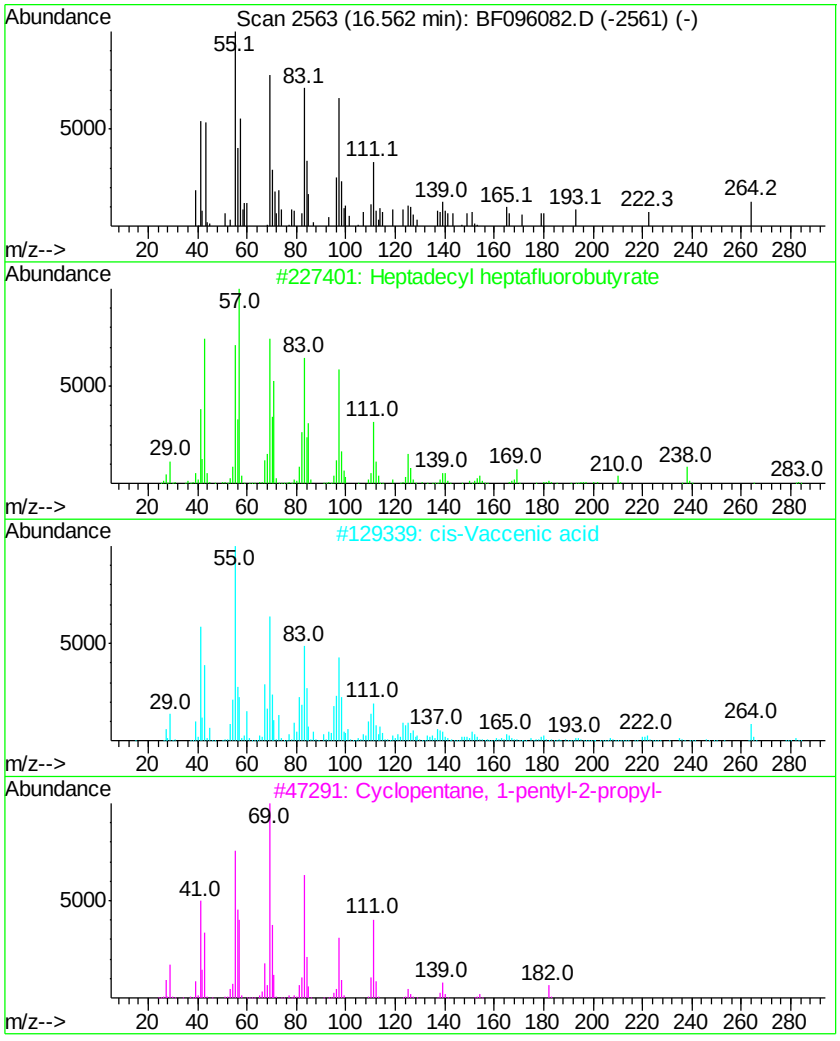
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

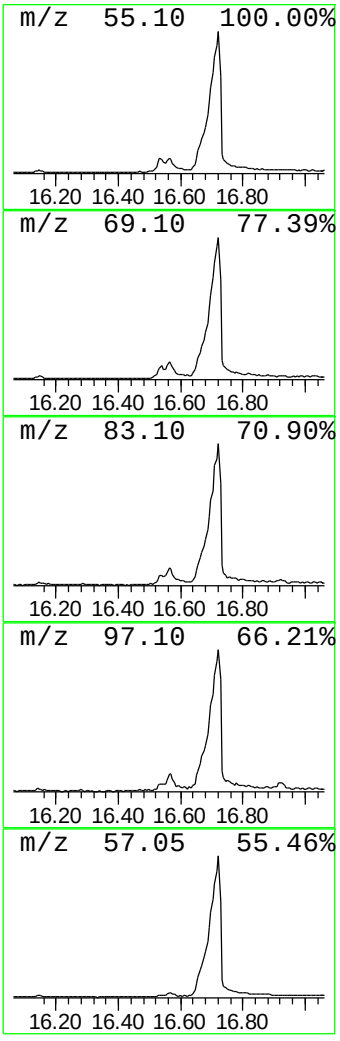
****

Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	6.06 ng	177893	Chrysene-d12	18.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	58
3	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	58
4	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	49
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	47





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TIC Library : C:\DATABASE\NIST11.L
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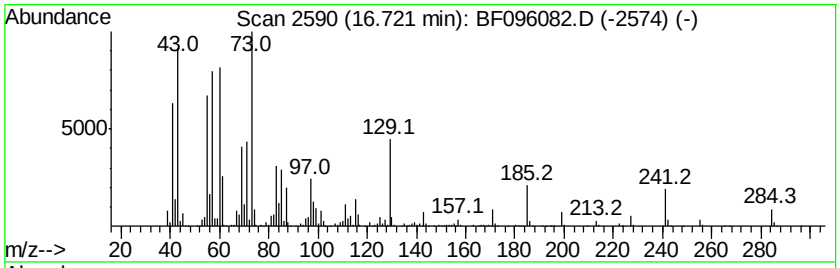
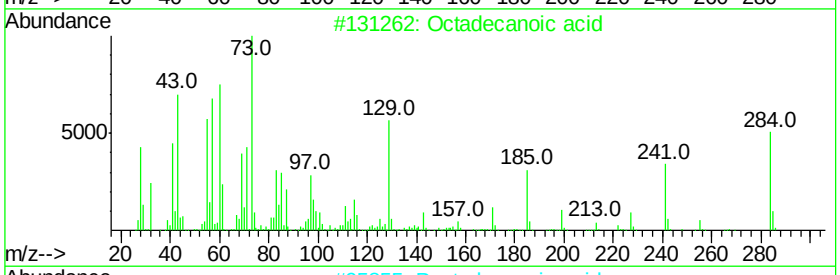
****

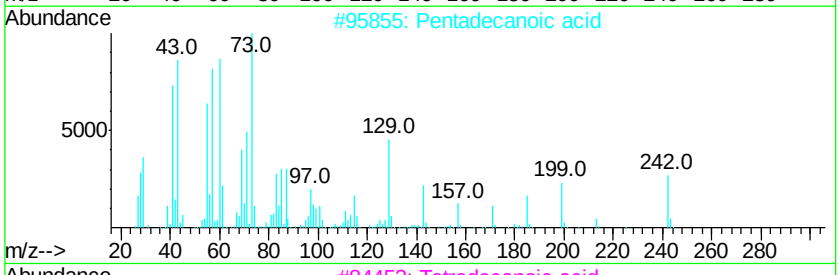
Peak Number 12 Octadecanoic acid Concentration Rank 1

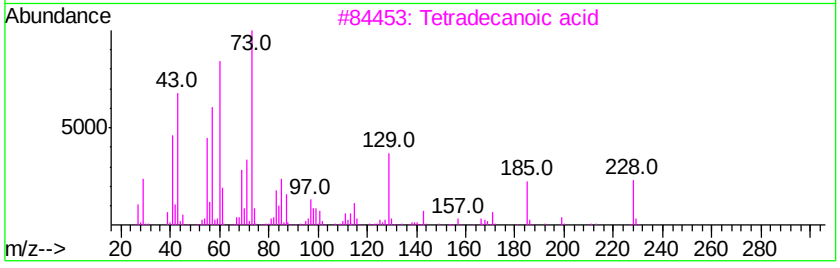
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	166.97 ng	4902020	Chrysene-d12	18.27

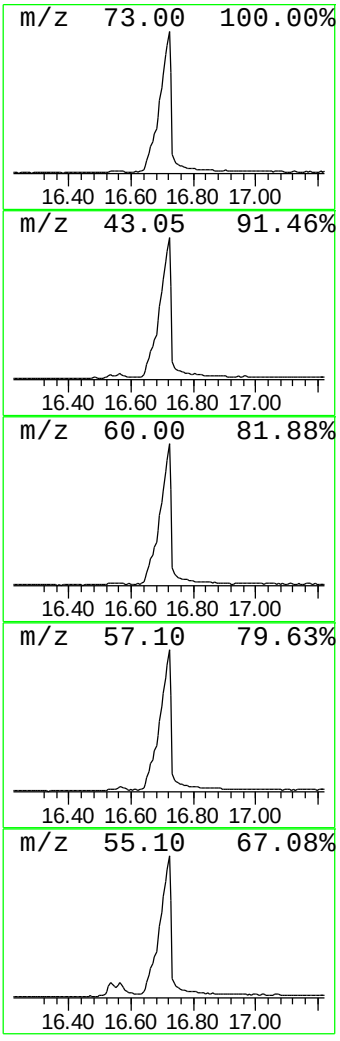
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062117\
Data File : BF096082.D
Acq On : 21 Jun 2017 13:55
Operator : SJ/MA
Sample : I3759-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-02-061617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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
4-Penten-2-one, 4...	2.37	3.1	ng	65796	1	7.29	422783	20.0
3-Penten-2-one, 4...	3.45	9.8	ng	206592	1	7.29	422783	20.0
2-Pentanone, 4-hy...	4.50	11.8	ng	249677	1	7.29	422783	20.0
unknown6.95	6.95	108.9	ng	2301220	1	7.29	422783	20.0
Nonanoic acid	12.71	3.7	ng	120163	3	12.14	643385	20.0
Tetradecanoic acid	14.22	2.9	ng	95672	4	14.53	667039	20.0
n-Hexadecanoic acid	15.60	67.3	ng	2243060	4	14.53	667039	20.0
9,12-Octadecadien...	16.54	10.0	ng	293485	5	18.27	587167	20.0
Heptadecyl heptaf...	16.56	6.1	ng	177893	5	18.27	587167	20.0
Octadecanoic acid	16.72	167.0	ng	4902020	5	18.27	587167	20.0