LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087335.D
Acq On : 24 May 2016 11:14
Operator : UM/SJ
Sample : H3168-14
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-12-COMP

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-BF052316.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	1.690	6	9	52	rVB	3039204	8770616	100.00%	20.443%
2	4.890	287	289	306	rBV	168300	449940	5.13%	1.049%
3	5.530	343	345	371	rBV	2198529	3494922	39.85%	8.146%
4	7.153	484	487	494	rBV	2446346	3635107	41.45%	8.473%
5	7.268	494	497	506	rVB	2561317	3651321	41.63%	8.511%
6	7.610	525	527	538	rVB	685331	923213	10.53%	2.152%
7	7.850	545	548	558	rBV	1707554	2673068	30.48%	6.230%
8	8.525	604	607	632	rBV	1617246	2474236	28.21%	5.767%
9	9.645	702	705	720	rBV	763706	1236235	14.10%	2.881%
10	11.417	857	860	863	rBV	2755575	3843984	43.83%	8.960%
11	12.114	919	921	925	rBV	210898	280457	3.20%	0.654%
12	12.468	949	952	967	rVB	1013832	1473009	16.79%	3.433%
13	13.302	1023	1025	1028	rVB	119993	138056	1.57%	0.322%
14	13.760	1062	1065	1072	rBV	1458778	2383281	27.17%	5.555%
15	14.080	1090	1093	1098	rBV	103974	173896	1.98%	0.405%
16	14.880	1160	1163	1172	rVB	806043	1303025	14.86%	3.037%
17	17.051	1351	1353	1356	rVB	206779	212977	2.43%	0.496%
18	17.211	1364	1367	1370	rBV	2931320	3236111	36.90%	7.543%
19	17.977	1431	1434	1437	rBV	138999	146451	1.67%	0.341%
20	18.514	1478	1481	1482	rVV	58580	125426	1.43%	0.292%
21	18.549	1482	1484	1487	rVV	621555	1085939	12.38%	2.531%
22	18.606	1487	1489	1492	rVB	150653	255378	2.91%	0.595%
23	19.577	1571	1574	1576	rBV	184626	226742	2.59%	0.528%
24	20.217	1628	1630	1636	rVV	503476	709851	8.09%	1.655%

Sum of corrected areas: 42903241

LSC Report - Integrated Chromatogram

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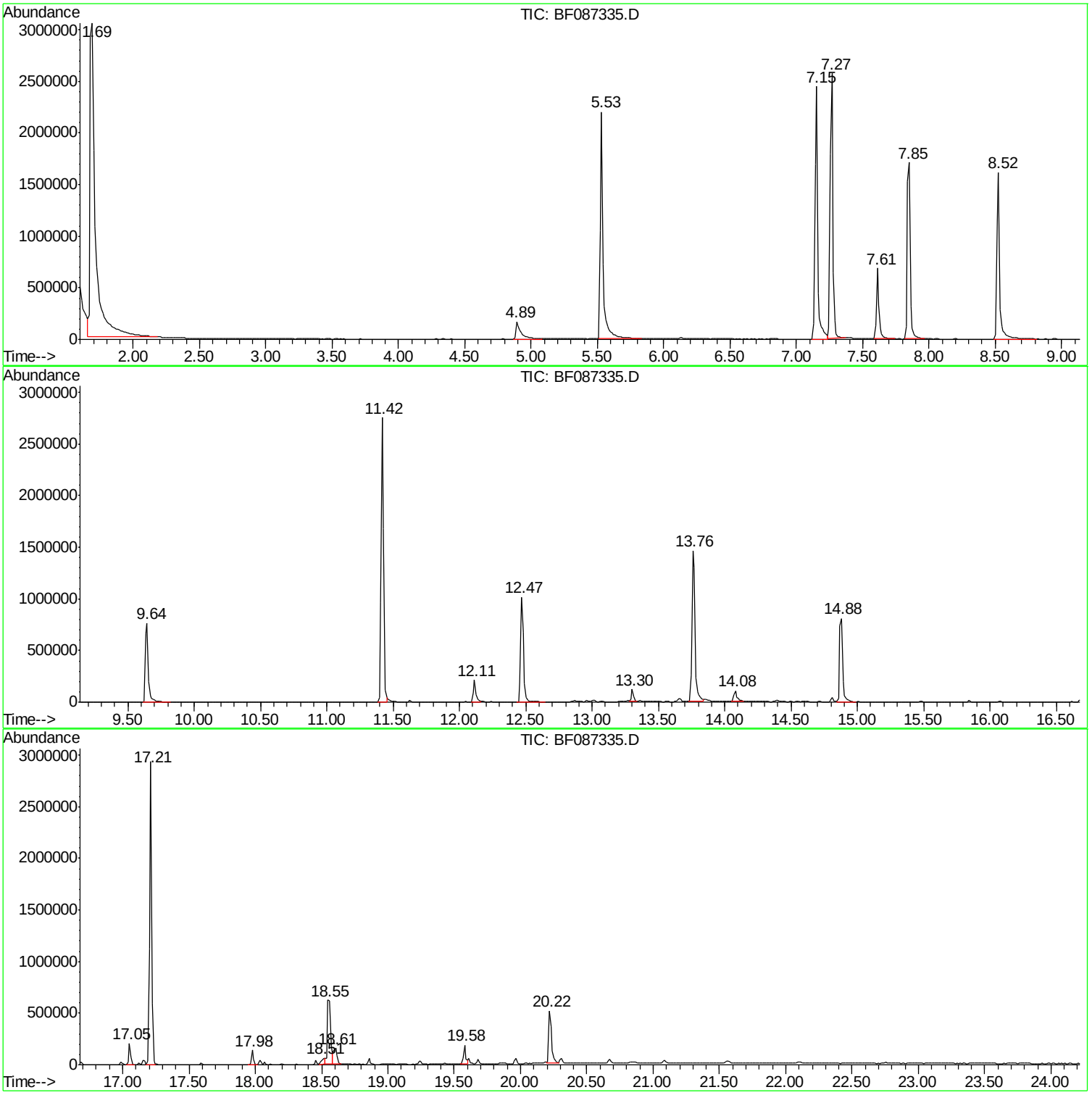
BNA_F
ClientSampleId :
SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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ClientSampleId : SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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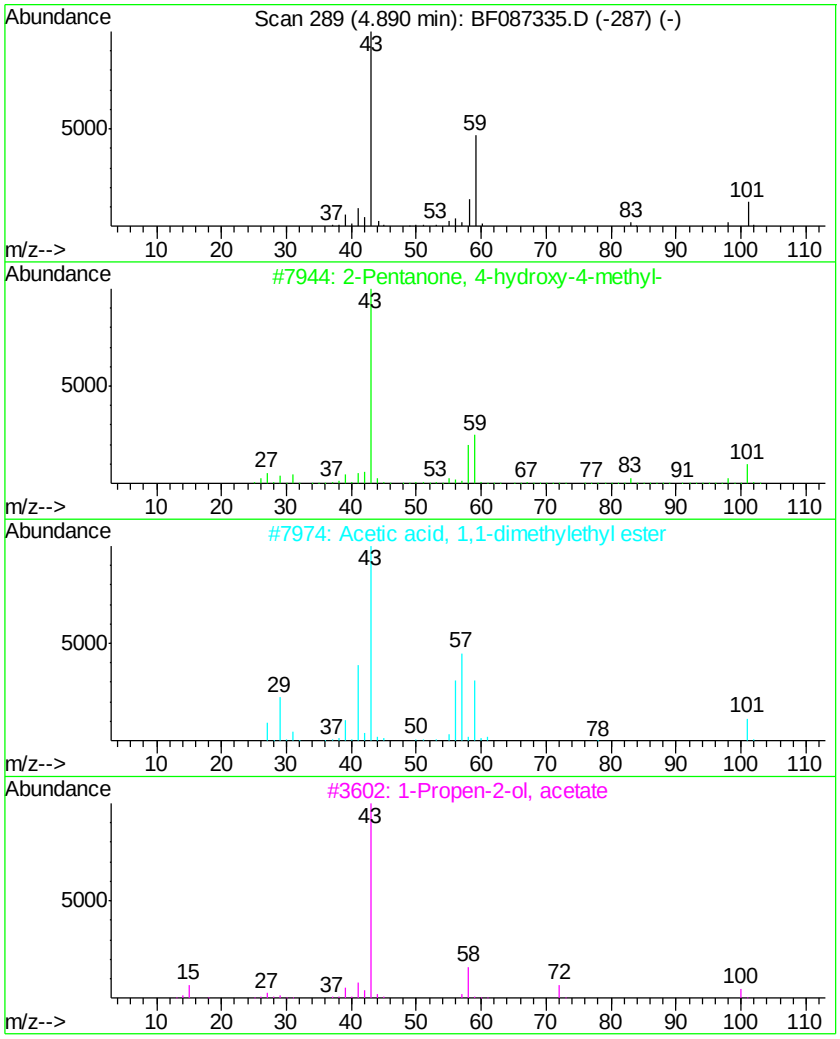
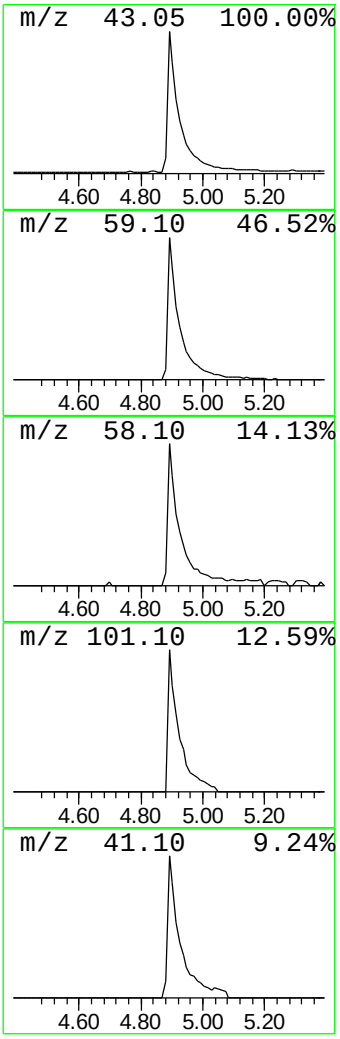
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	9.75 ng	449940	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
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Sample : H3168-14
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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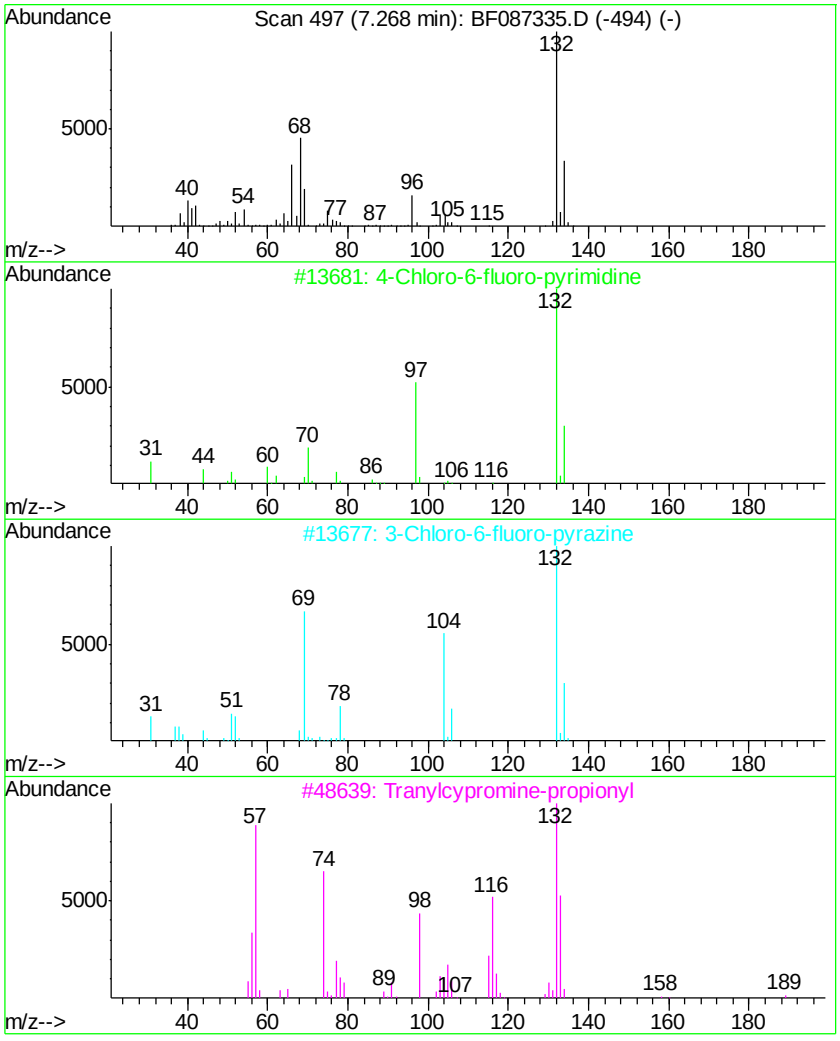
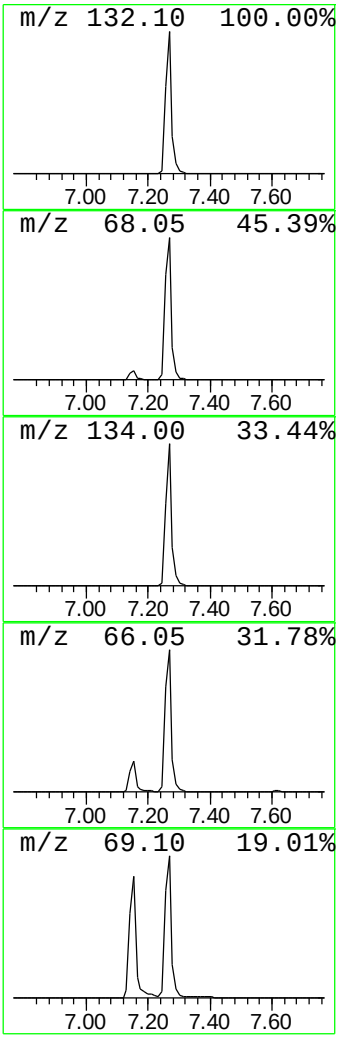
Peak Number 3 unknown7.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	79.10 ng	3651320	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Sample : H3168-14
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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TIC Library : C:\DATABASE\NIST02.L
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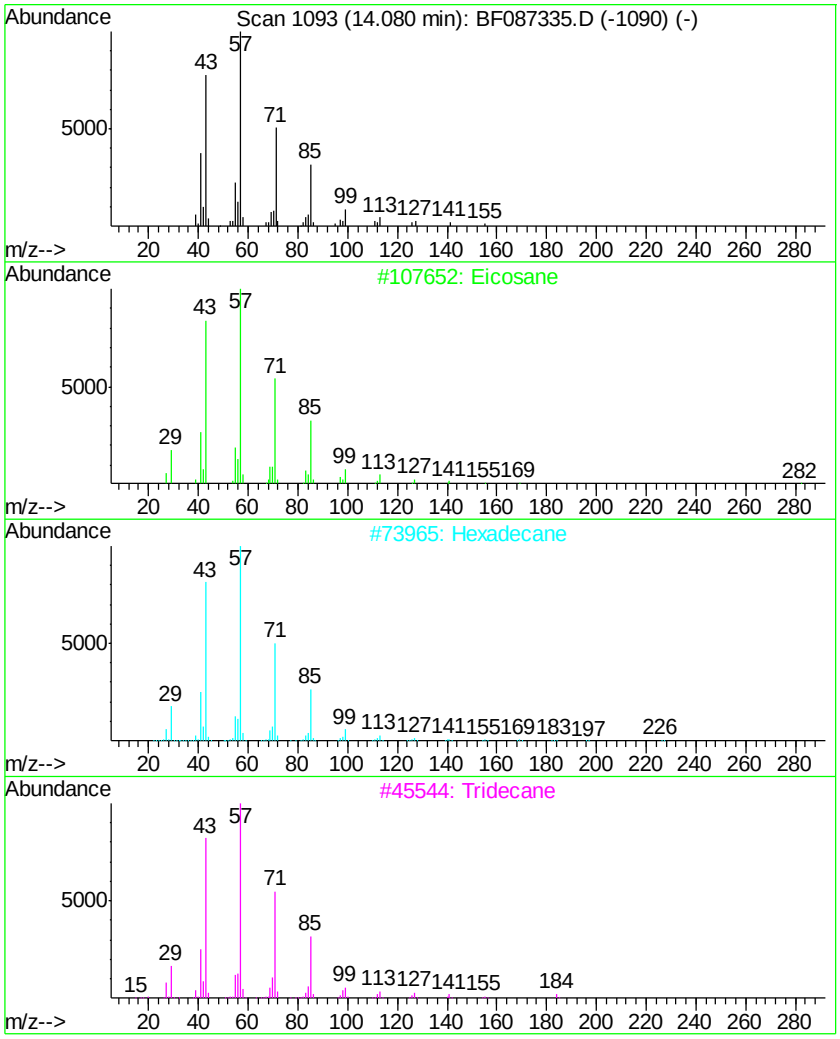
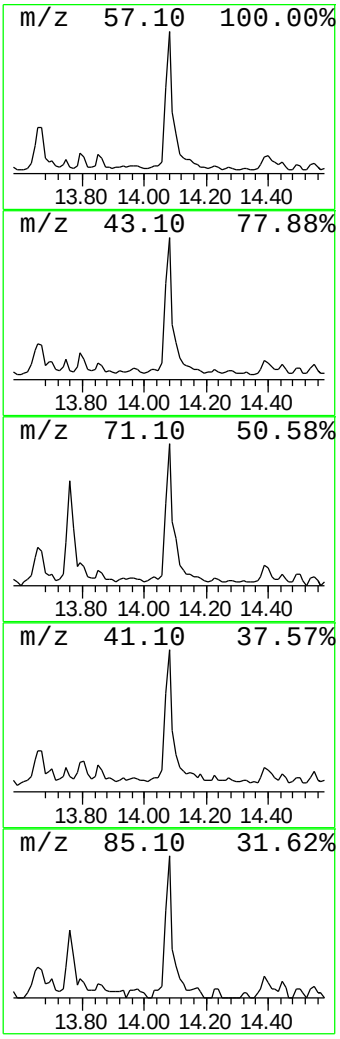
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.67 ng	173896	Phenanthrene-d10	14.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	86
4	Decane, 3-bromo-	220	C10H21Br	030571-71-2	80
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78





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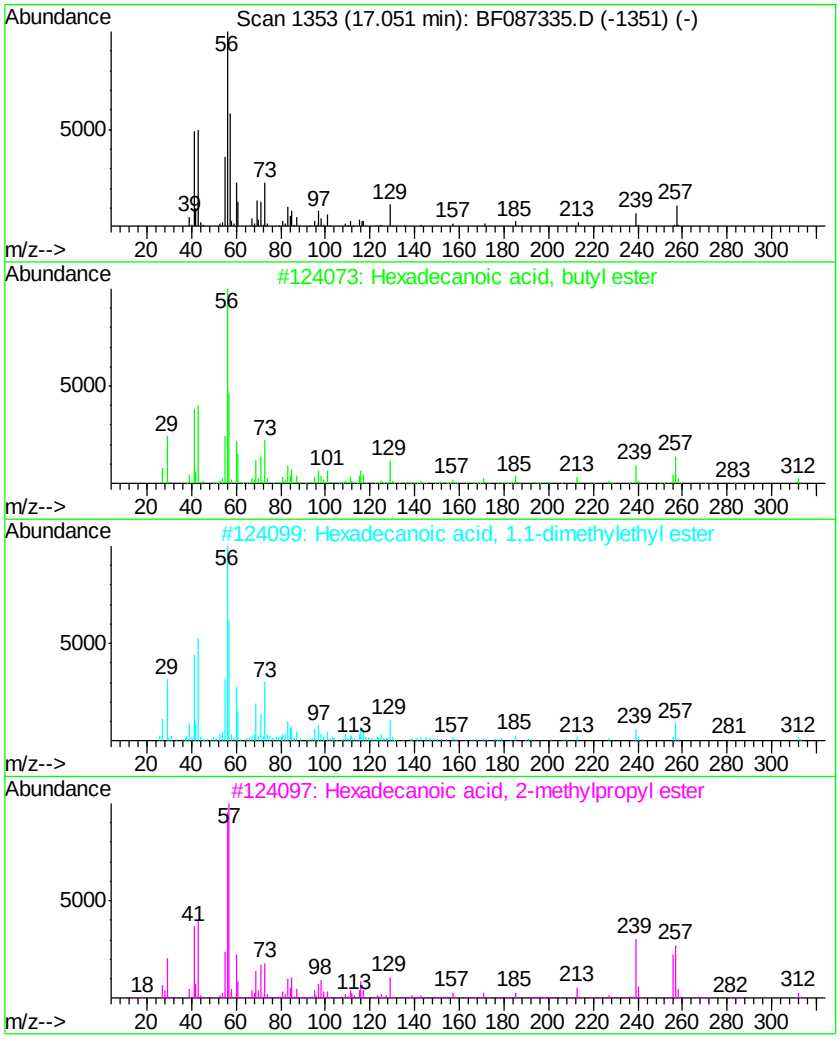
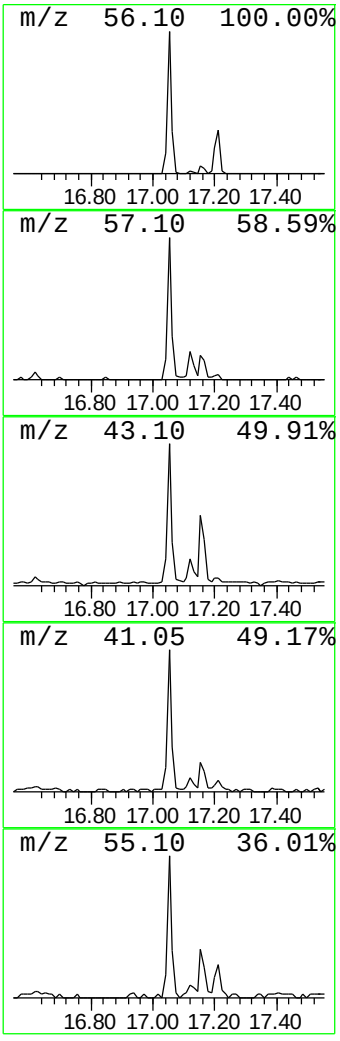
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	3.92 ng	212977	Chrysene-d12	18.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37





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ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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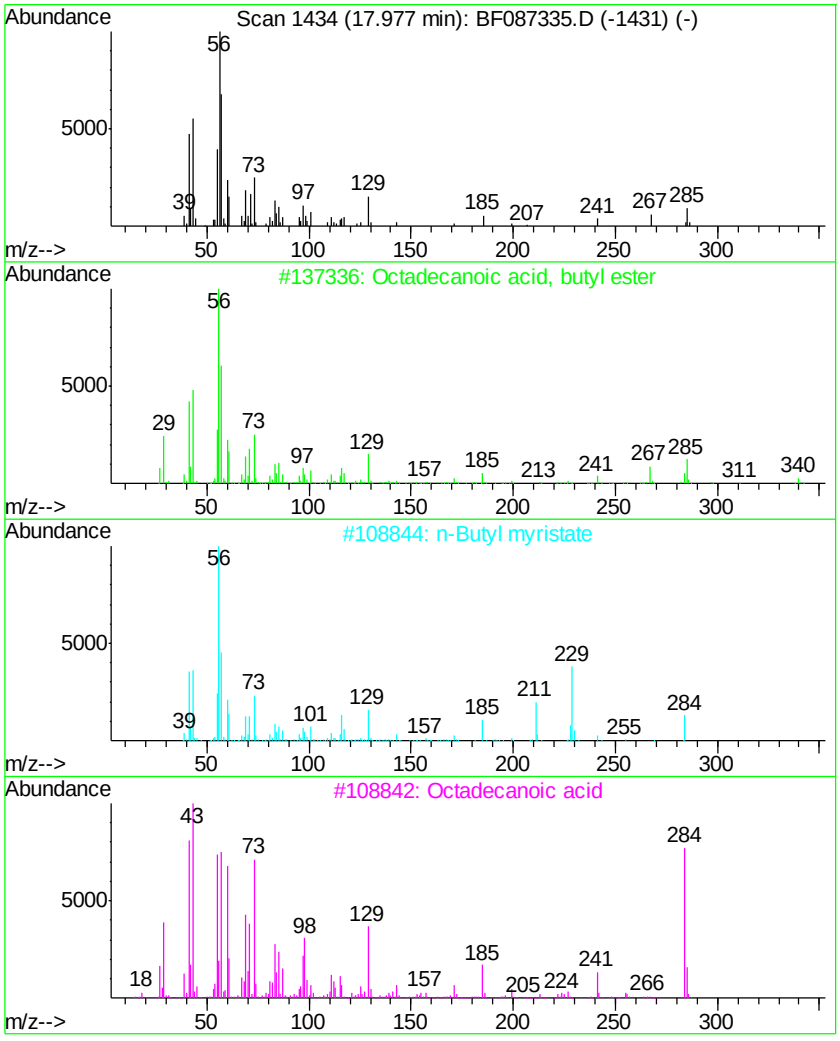
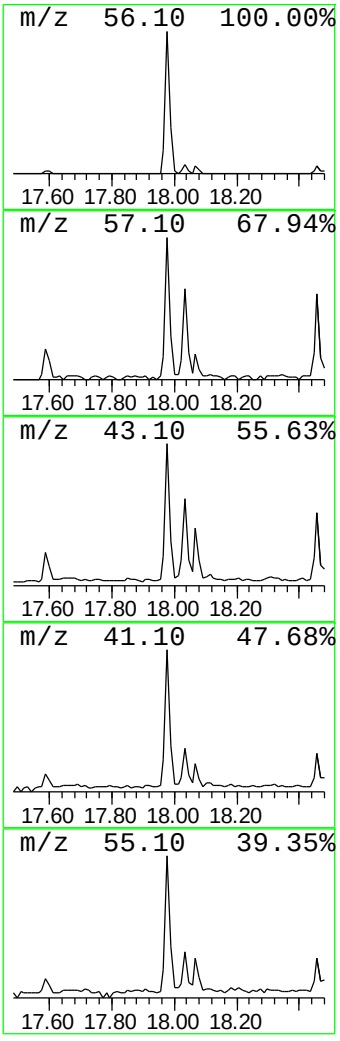
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	2.70 ng	146451	Chrysene-d12	18.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	86
3	Octadecanoic acid	284	C18H36O2	000057-11-4	43
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35





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

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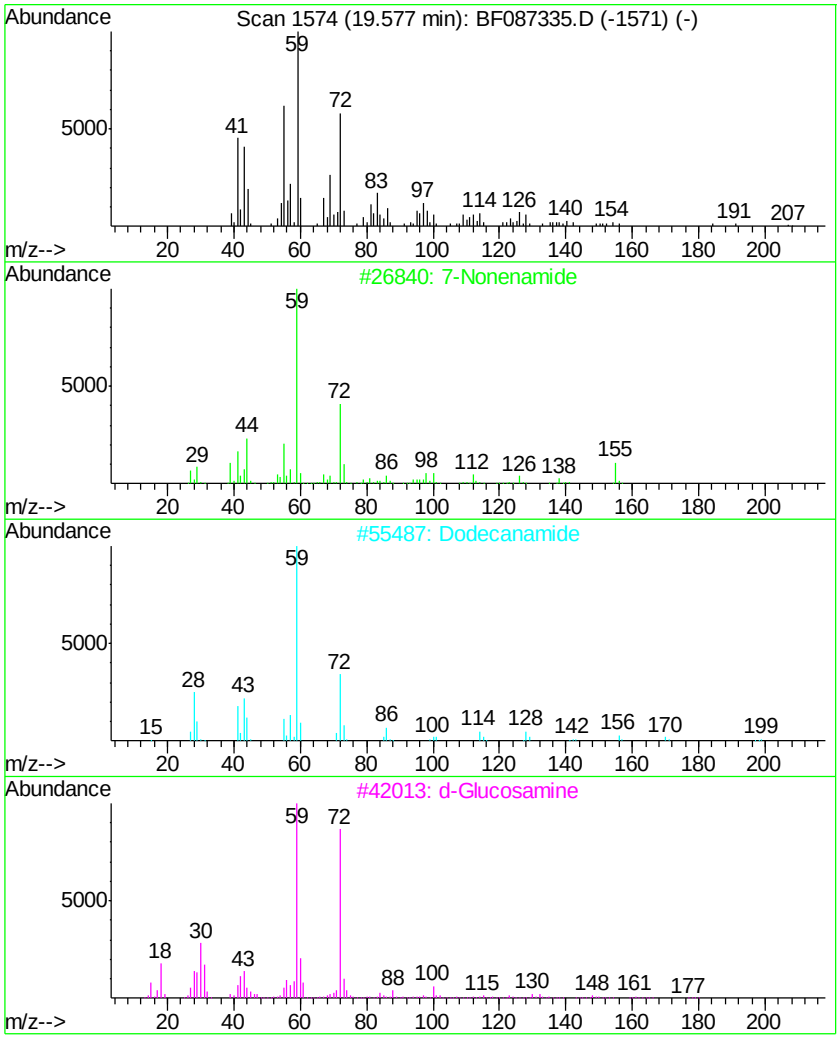
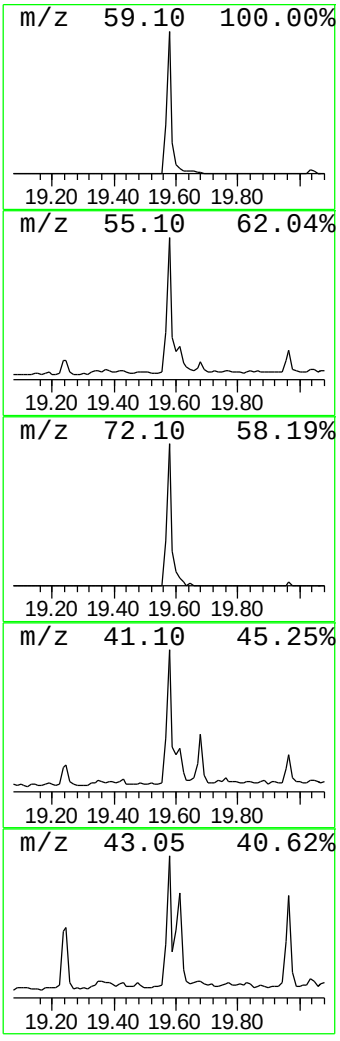
Peak Number 8 7-Nonenamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.58	6.39 ng	226742	Perylene-d12	20.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide	155	C9H17NO	090949-53-4	53
2	Dodecanamide	199	C12H25NO	001120-16-7	53
3	d-Glucosamine	179	C6H13NO5	000090-77-7	53
4	Hexanamide	115	C6H13NO	000628-02-4	50
5	Mannosamine hydrochloride	179	C6H13NO5	1000127-68-8	47





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	9.8	ng	449940	1	7.61	923213	20.0
unknown7.27	7.27	79.1	ng	3651320	1	7.61	923213	20.0
Eicosane	14.08	2.7	ng	173896	4	14.88	1303030	20.0
Hexadecanoic acid...	17.05	3.9	ng	212977	5	18.56	1085940	20.0
Octadecanoic acid...	17.98	2.7	ng	146451	5	18.56	1085940	20.0
7-Nonenamide	19.58	6.4	ng	226742	6	20.22	709851	20.0