LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090183.D
Acq On : 22 Sep 2016 2:28
Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

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-BF092016.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	1.667	6	7	58	rVB	1729622	4600774	100.00%	20.453%
2	4.593	260	263	275	rBV	190232	285807	6.21%	1.271%
3	5.073	302	305	307	rBV	1174044	1412019	30.69%	6.277%
4	6.159	398	400	403	rBV	984363	1316261	28.61%	5.852%
5	6.273	408	410	413	rVV	1635205	1479207	32.15%	6.576%
6	6.502	428	430	433	rBV	491099	672141	14.61%	2.988%
7	6.662	442	444	446	rBV	1451841	1252348	27.22%	5.567%
8	7.073	478	480	483	rBV	778654	798906	17.36%	3.552%
9	7.793	541	543	546	rBV	1147928	993804	21.60%	4.418%
10	8.879	635	638	640	rBV	1854183	1878046	40.82%	8.349%
11	9.279	671	673	675	rBV	220544	234708	5.10%	1.043%
12	9.542	694	696	698	rBV	948418	973070	21.15%	4.326%
13	10.319	761	764	767	rBV	917453	873866	18.99%	3.885%
14	10.468	775	777	782	rBV	50045	58227	1.27%	0.259%
15	11.005	822	824	828	rBV	983366	885674	19.25%	3.937%
16	11.565	871	873	877	rBV2	57991	91125	1.98%	0.405%
17	12.594	960	963	965	rBV	1053752	1356979	29.49%	6.033%
18	13.074	1002	1005	1008	rBV	603346	579361	12.59%	2.576%
19	13.508	1040	1043	1046	rBV3	234648	409102	8.89%	1.819%
20	13.622	1050	1053	1056	rBV	721729	938470	20.40%	4.172%
21	14.091	1092	1094	1096	rBV	121652	131429	2.86%	0.584%
22	14.137	1096	1098	1101	rBV3	98968	199086	4.33%	0.885%
23	14.948	1167	1169	1171	rBV	445917	485179	10.55%	2.157%
24	15.371	1203	1206	1211	rBV3	143703	372611	8.10%	1.656%
25	15.863	1247	1249	1254	rVB	127097	216144	4.70%	0.961%

Sum of corrected areas: 22494344

LSC Report - Integrated Chromatogram

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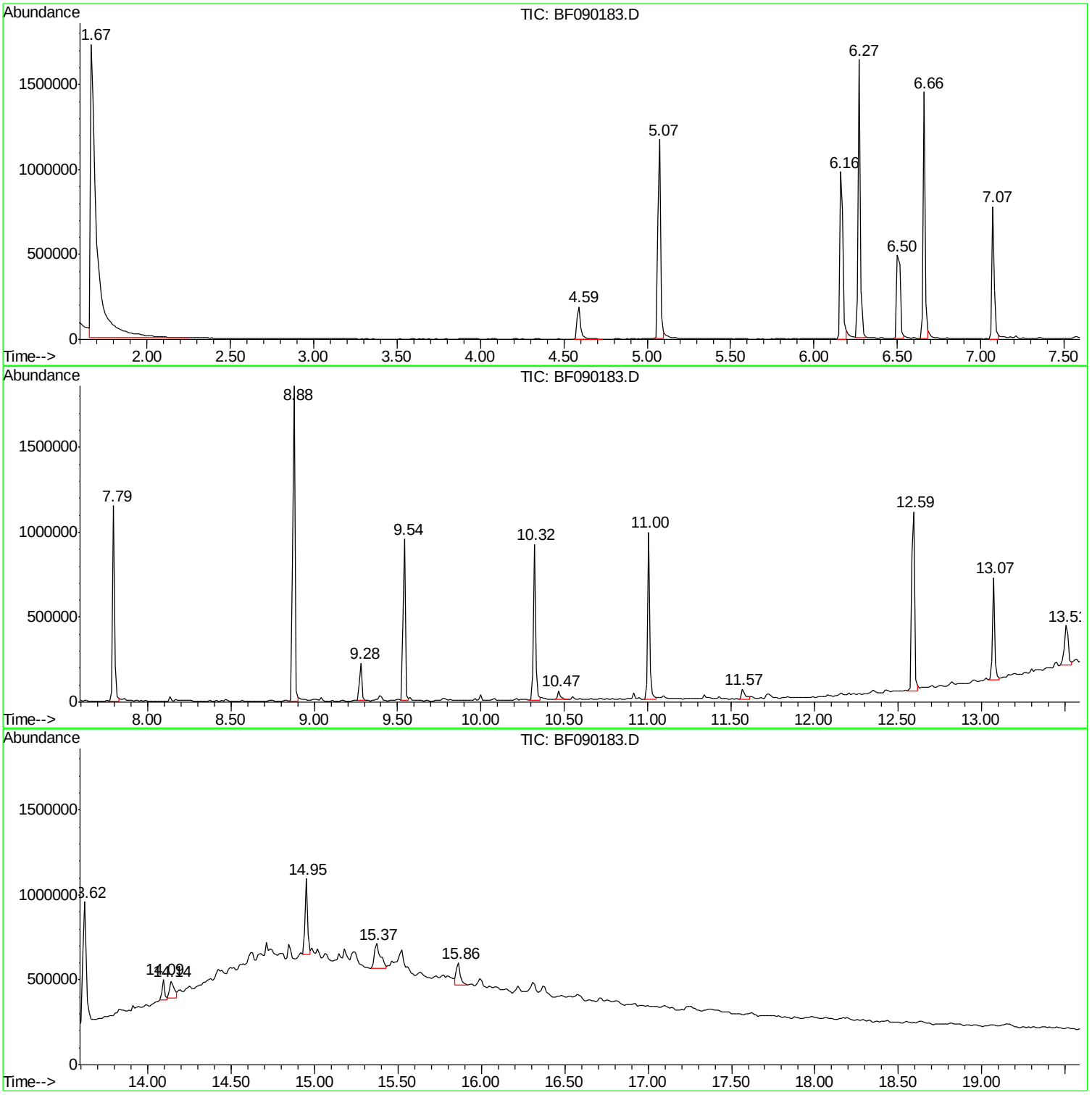
Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090183.D
Acq On : 22 Sep 2016 2:28
Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

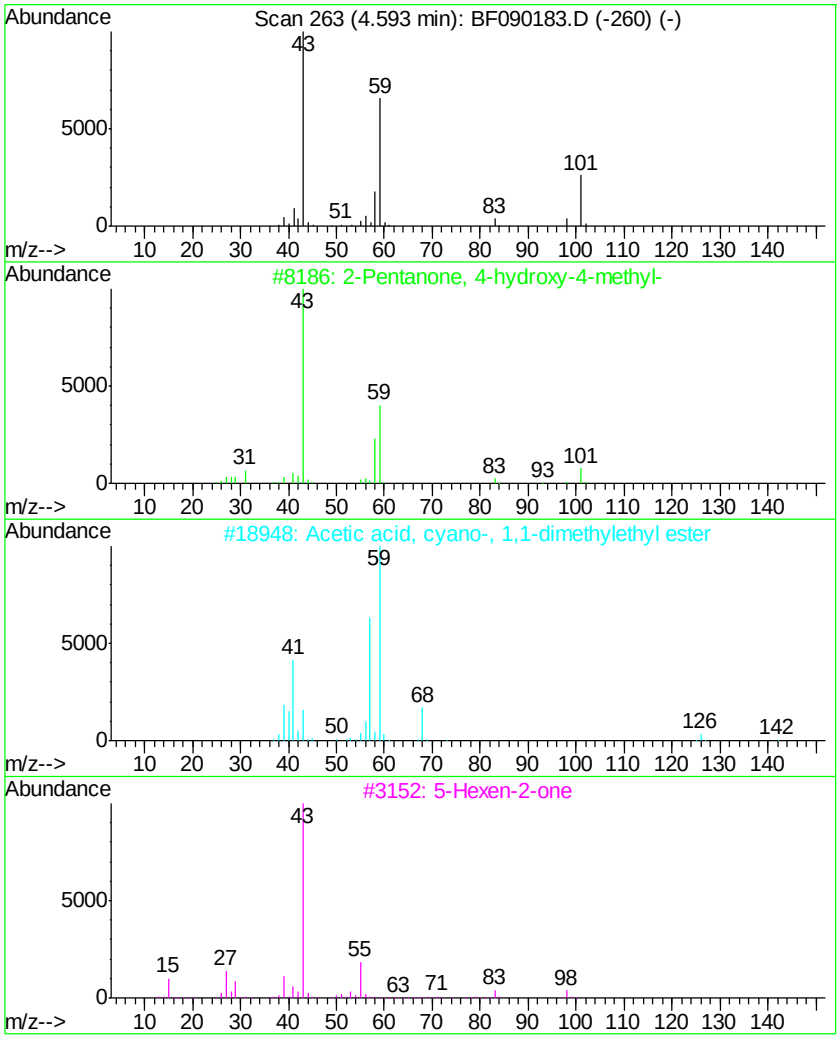
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

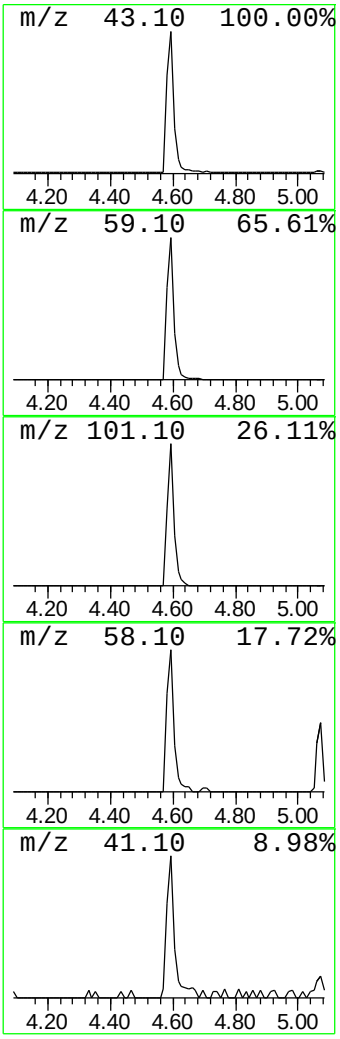
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	8.50 ng	285807	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

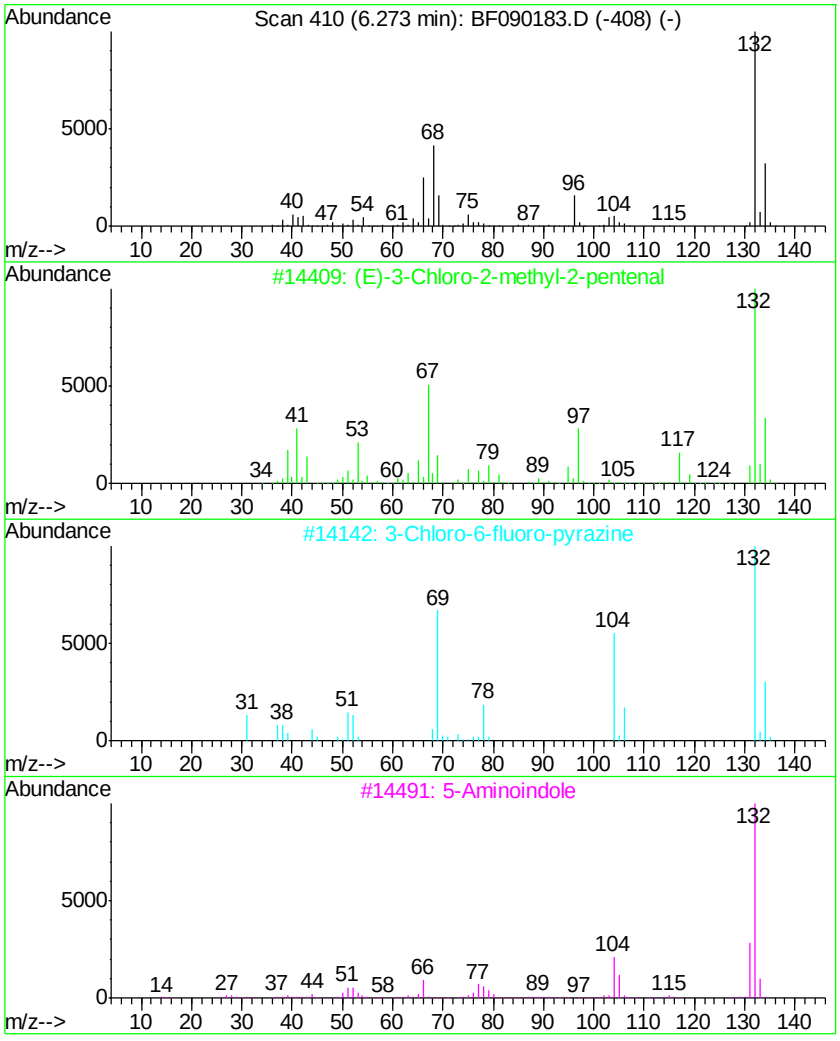
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

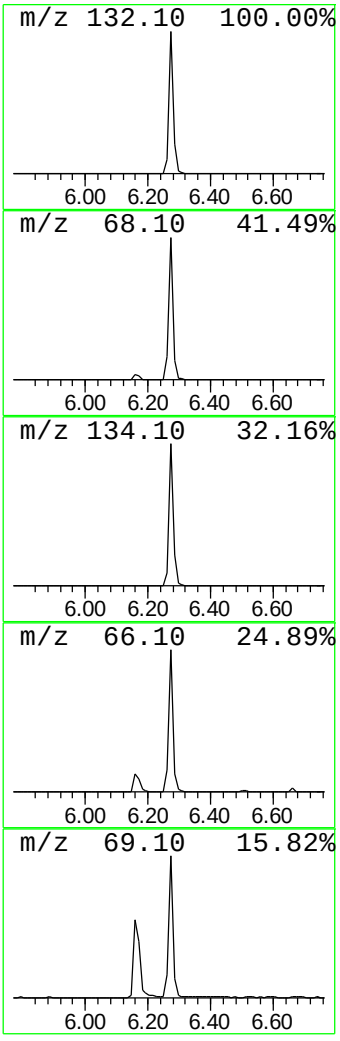
****

Peak Number 3 unknown6.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	44.01 ng	1479210	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090183.D
Acq On : 22 Sep 2016 2:28
Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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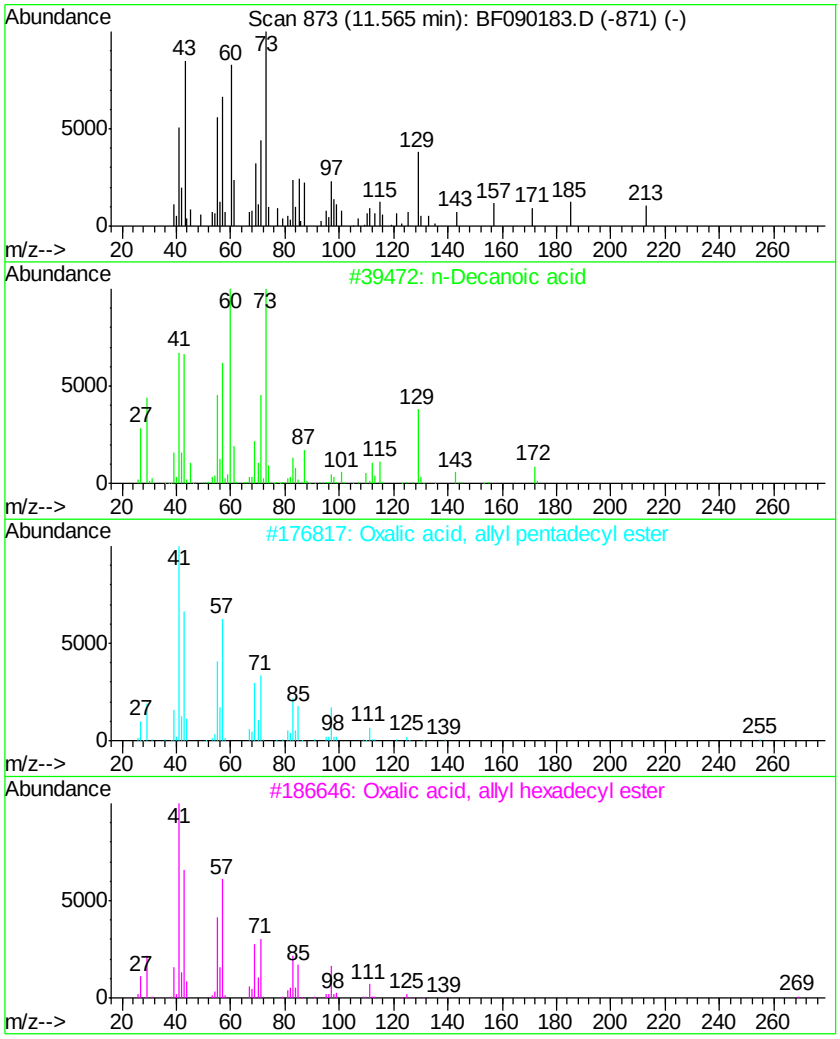
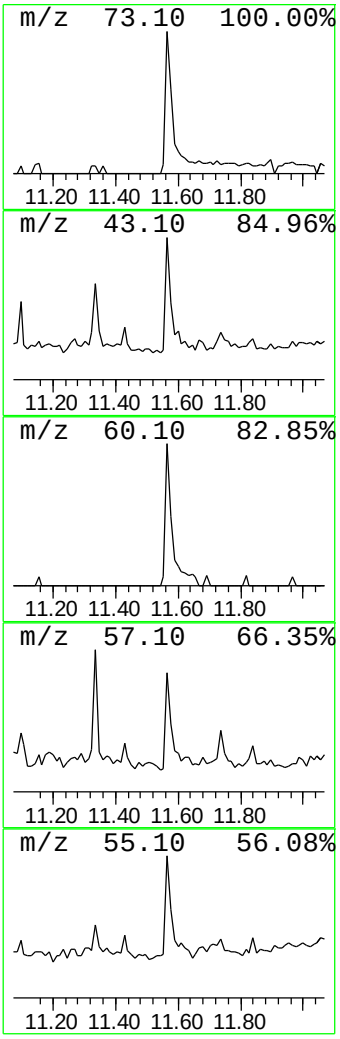
Peak Number 5 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	2.06 ng	91125	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	59
2	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18
3	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	18
4	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	14
5	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	10





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Acq On : 22 Sep 2016 2:28
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Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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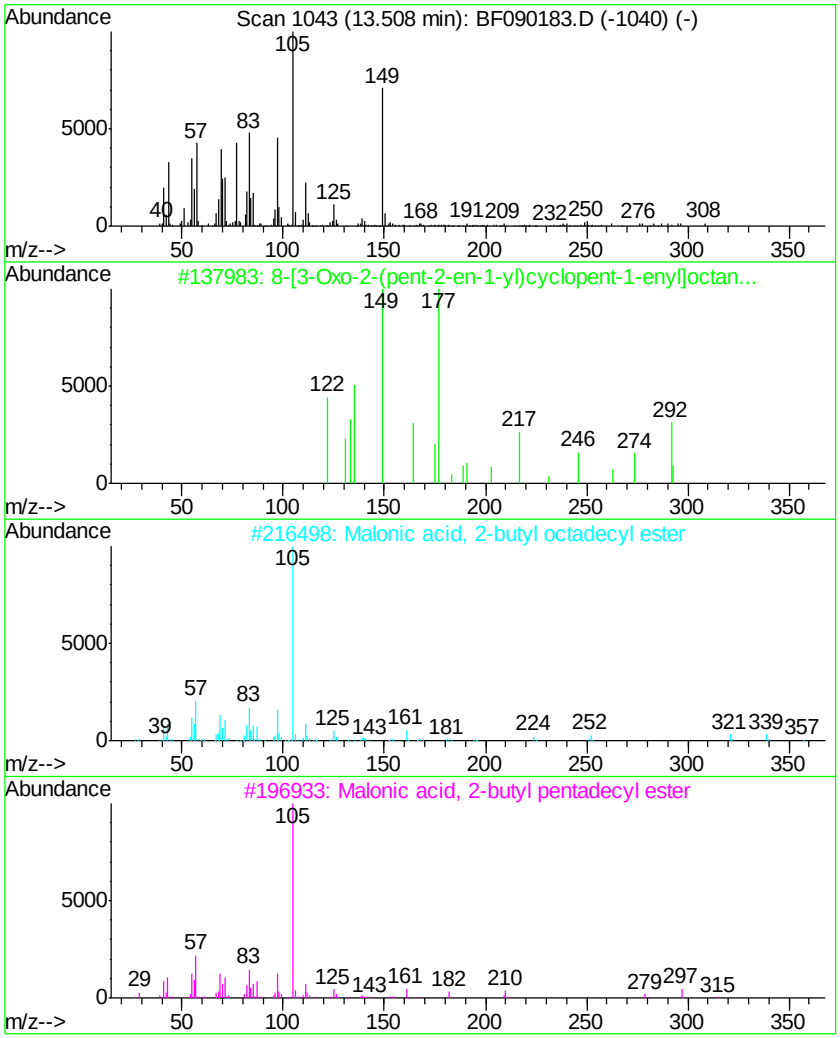
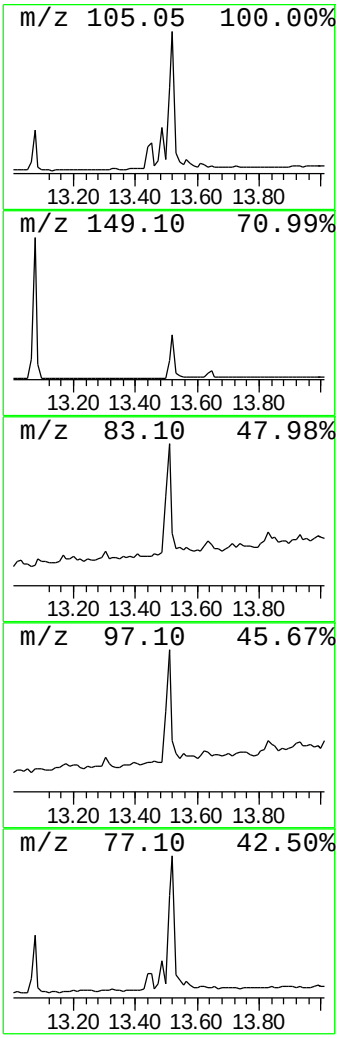
Peak Number 6 8-[3-Oxo-2-(pent-2-en-1-yl)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	8.72 ng	409102	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-[3-Oxo-2-(pent-2-en-1-yl)cyclo...	292	C18H28O3	1000105-21-8	81
2	Malonic acid, 2-butyl octadecyl ...	412	C25H48O4	1000349-08-4	43
3	Malonic acid, 2-butyl pentadecyl...	370	C22H42O4	1000349-08-0	22
4	Malonic acid, 2-decyl undecyl ester	398	C24H46O4	1000349-09-6	14
5	1,4-Butanedione, 1,4-diphenyl-	238	C16H14O2	000495-71-6	11





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Acq On : 22 Sep 2016 2:28
Operator : UM/SJ
Sample : H4856-15 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

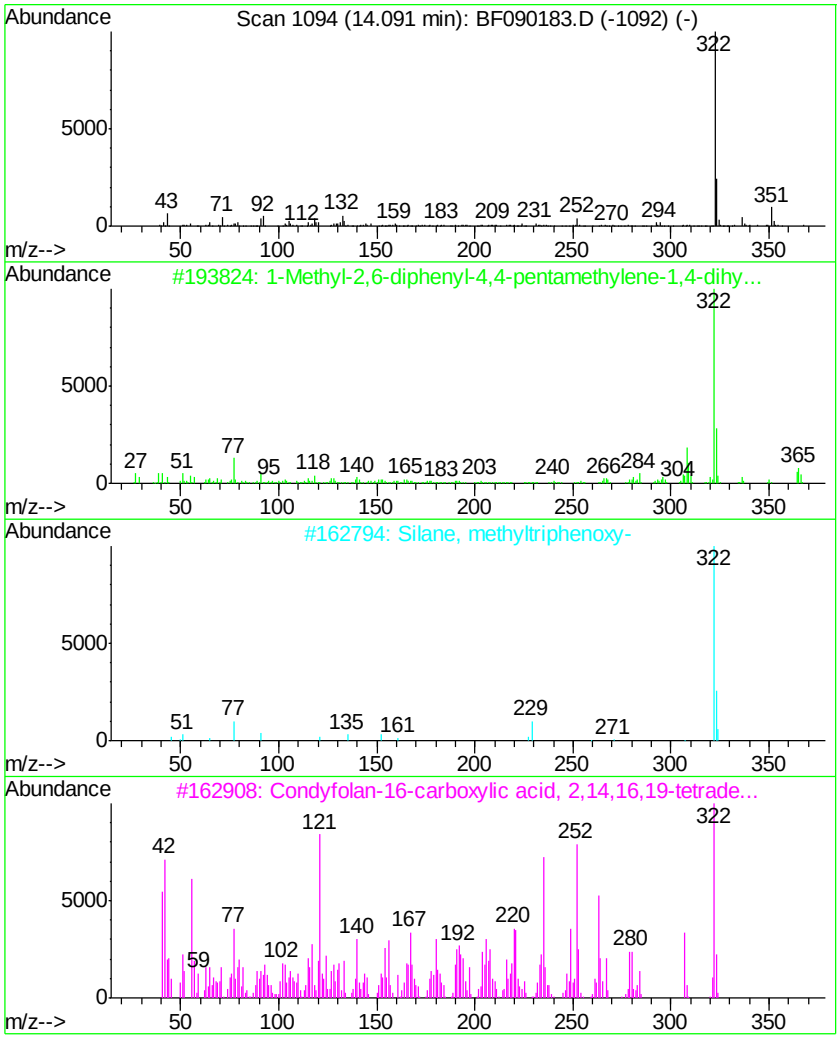
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

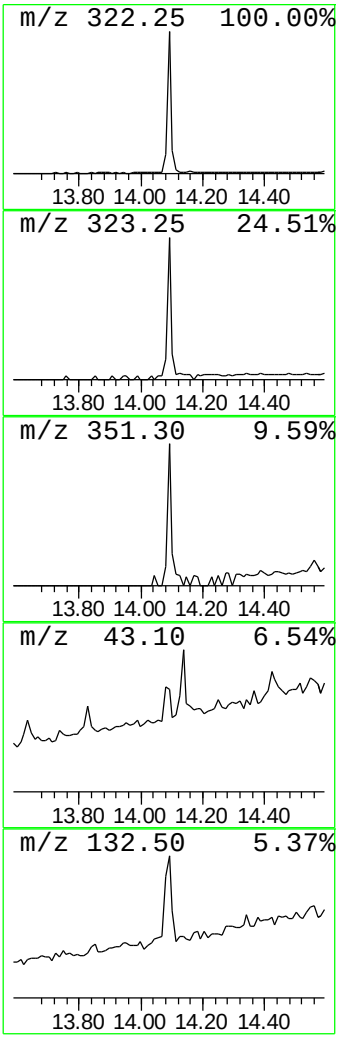
****

Peak Number 7 1-Methyl-2,6-diphenyl-4,4-p... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	2.80 ng	131429	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2,6-diphenyl-4,4-pentam...	365	C25H23N3	083078-31-3	64
2	Silane, methyltriphenoxy-	322	C19H18O3Si	003439-97-2	59
3	Condyfolan-16-carboxylic acid, 2...	322	C20H22N2O2	004939-81-5	50
4	3-Pyrazolin-5-one, 4-butyl-1,2-d...	322	C20H22N2O2	027258-01-1	45
5	1H-Indole, 3-Phenyl-2-(3'-methyl...	322	C23H18N2	164936-86-1	45





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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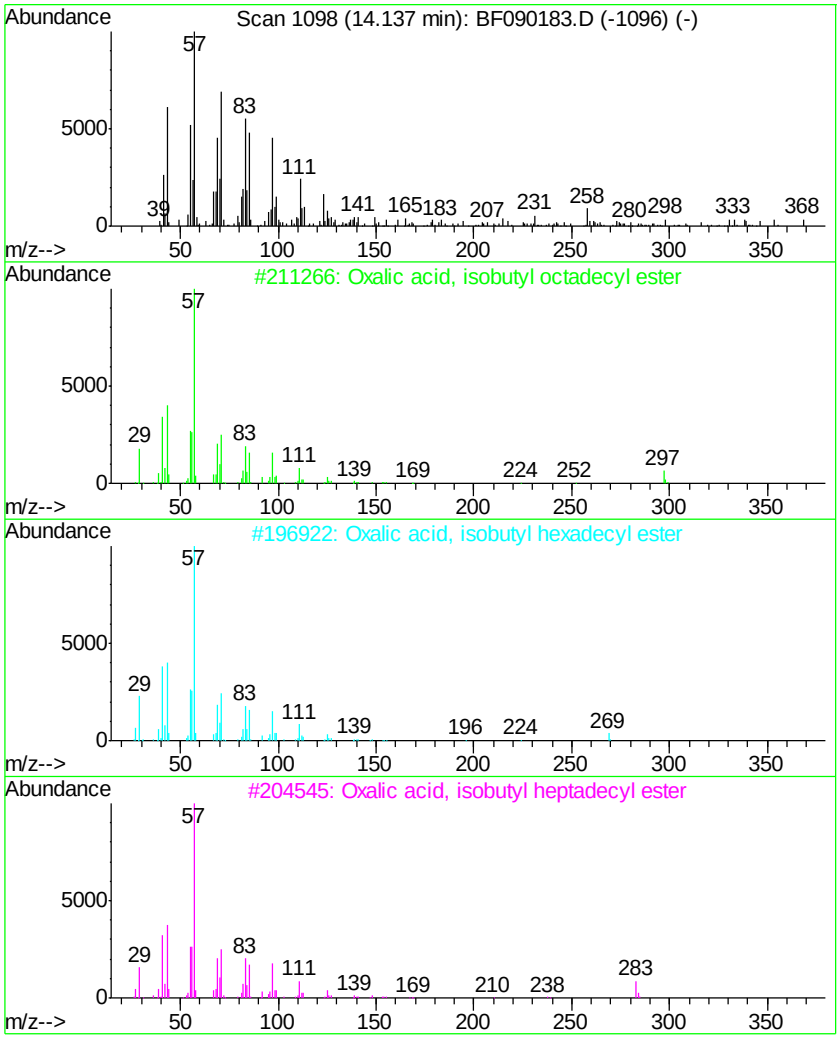
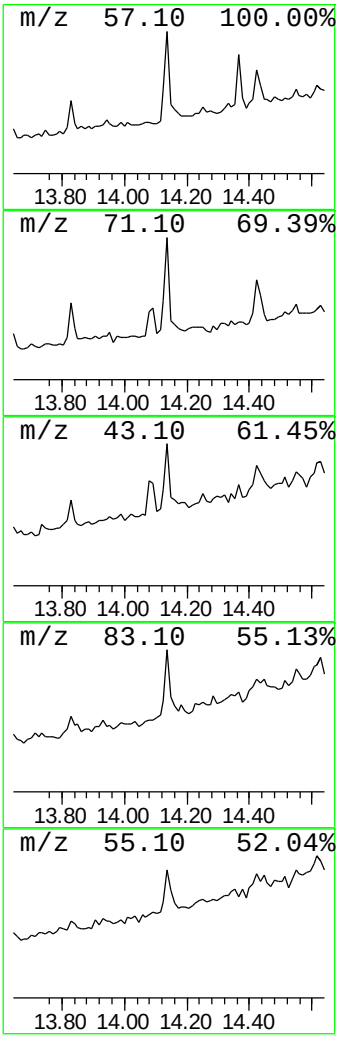
Peak Number 8 Oxalic acid, isobutyl octad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	4.24 ng	199086	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	81
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	74
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	64
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	60





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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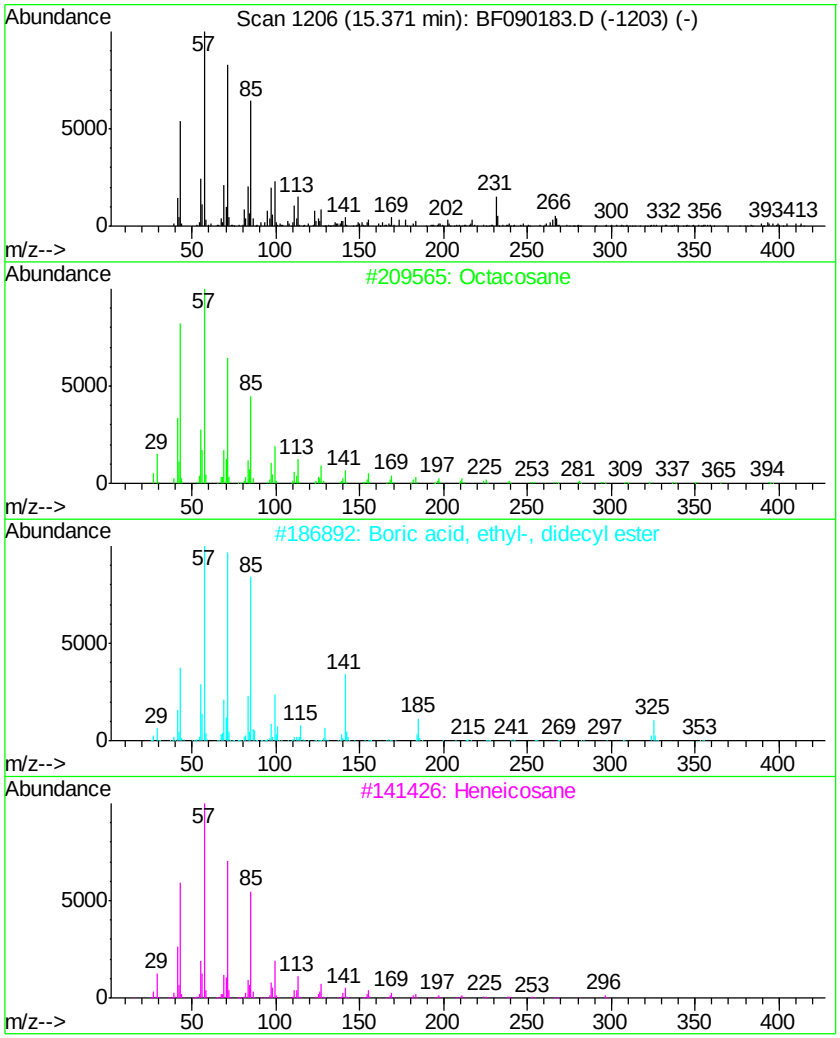
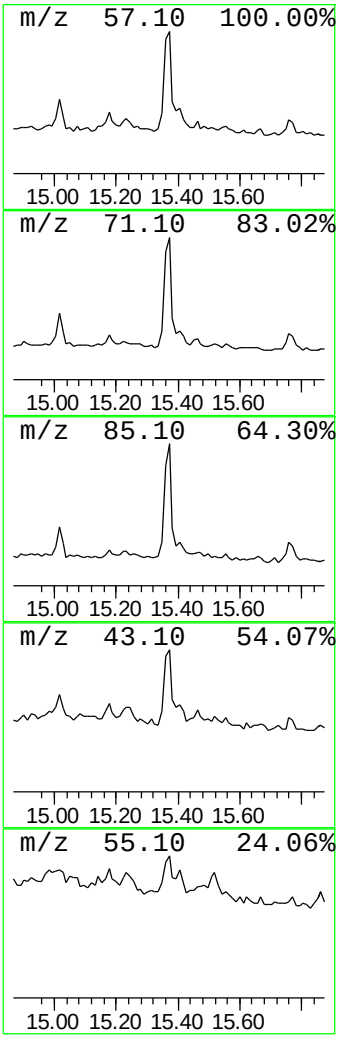
Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	15.36 ng	372611	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	72
2	Boric acid, ethyl-, didecyl ester	354	C22H47BO2	1000152-34-4	68
3	Heneicosane	296	C21H44	000629-94-7	64
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	64





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

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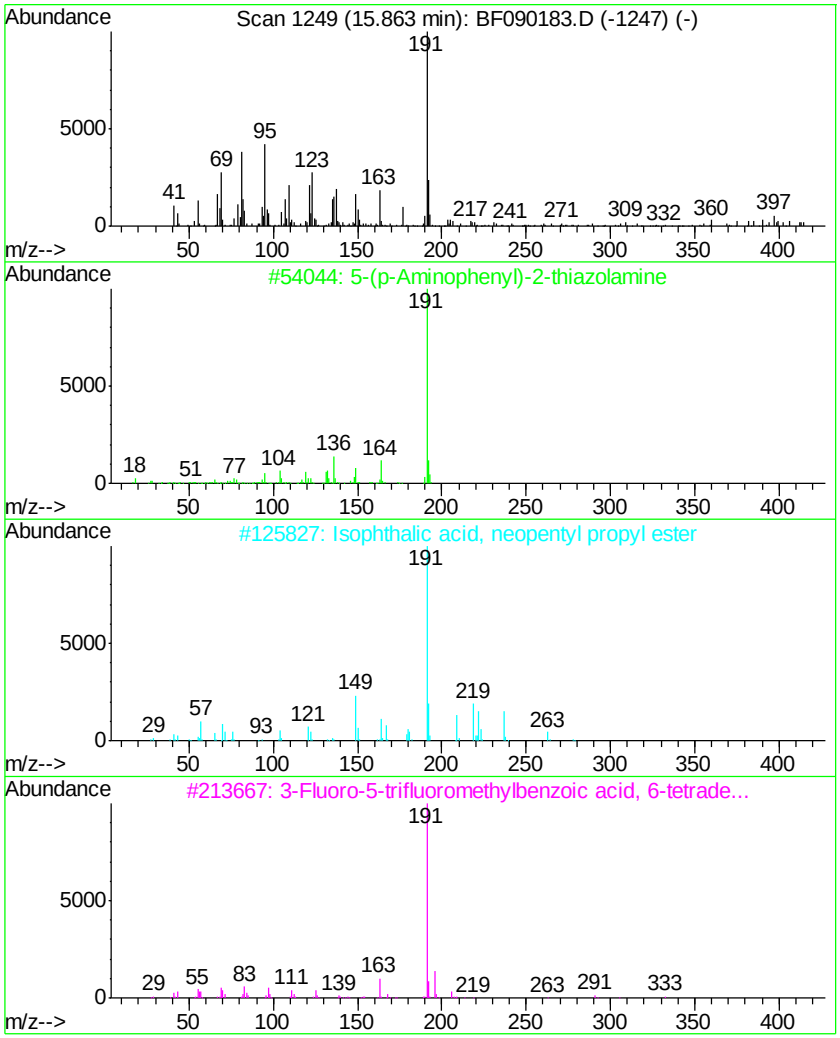
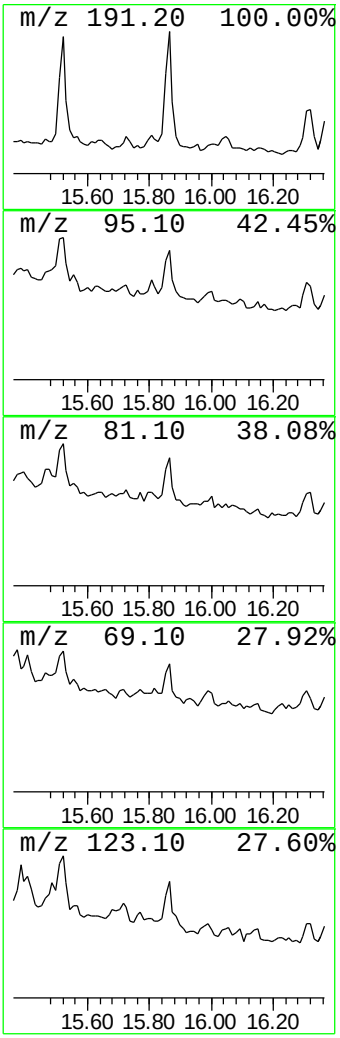
Peak Number 10 unknown15.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	8.91 ng	216144	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35
2	Isophthalic acid, neopentyl prop...	278	C16H22O4	1000343-85-9	35
3	3-Fluoro-5-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-66-7	27
4	4-Fluoro-3-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-68-7	27
5	2-Fluoro-3-trifluoromethylbenzoi...	376	C20H28F4O2	1000338-51-1	27





Tentatively Identified Compound (LSC) summary

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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...	4.59	8.5	ng	285807	1	6.51	672141	20.0
unknown6.27	6.27	44.0	ng	1479210	1	6.51	672141	20.0
n-Decanoic acid	11.57	2.1	ng	91125	4	11.00	885674	20.0
8-[3-Oxo-2-(pent-...	13.51	8.7	ng	409102	5	13.62	938470	20.0
1-Methyl-2,6-diph...	14.09	2.8	ng	131429	5	13.62	938470	20.0
Oxalic acid, isob...	14.14	4.2	ng	199086	5	13.62	938470	20.0
Octacosane	15.37	15.4	ng	372611	6	14.95	485179	20.0
unknown15.86	15.86	8.9	ng	216144	6	14.95	485179	20.0