LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090449.D
Acq On : 7 Oct 2016 17:16
Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

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-BF100516.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	5.194	247	250	253	rBV	907778	1087478	5.82%	1.106%
2	5.606	283	286	289	rBV	4031198	4597676	24.59%	4.674%
3	6.623	372	375	377	rBV	4641061	4678050	25.02%	4.756%
4	6.760	384	387	389	rBV	5562751	5281091	28.25%	5.369%
5	6.989	404	407	409	rBV	1617781	1474812	7.89%	1.499%
6	7.149	418	421	423	rVB	3051789	3807977	20.37%	3.871%
7	7.549	453	456	458	rBV	3211139	3172549	16.97%	3.225%
8	8.280	517	520	522	rBV	1508314	2034202	10.88%	2.068%
9	9.355	611	614	616	rBV	6144589	5590278	29.90%	5.683%
10	10.040	671	674	676	rVB	2535502	2438076	13.04%	2.479%
11	10.829	740	743	745	rBV	3797134	3504184	18.74%	3.562%
12	11.526	802	804	807	rVB	2623821	2211477	11.83%	2.248%
13	13.115	941	943	946	rBV	4130429	5507751	29.46%	5.599%
14	14.178	1033	1036	1038	rBV	1433429	1566984	8.38%	1.593%
15	14.567	1066	1070	1072	rBV	266923	648835	3.47%	0.660%
16	14.612	1072	1074	1076	rBV2	297953	599452	3.21%	0.609%
17	14.978	1095	1106	1107	rBV	1383377	5737102	30.68%	5.832%
18	15.047	1107	1112	1115	rVV	2668868	11121023	59.48%	11.306%
19	15.138	1117	1120	1123	rVV	2844793	10228459	54.71%	10.398%
20	15.218	1123	1127	1153	rVB	4168500	18697328	100.00%	19.008%
21	15.675	1164	1167	1169	rVB	982899	1253770	6.71%	1.275%
22	15.835	1174	1181	1206	rVB2	428264	3129557	16.74%	3.181%

Sum of corrected areas: 98368111

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090449.D
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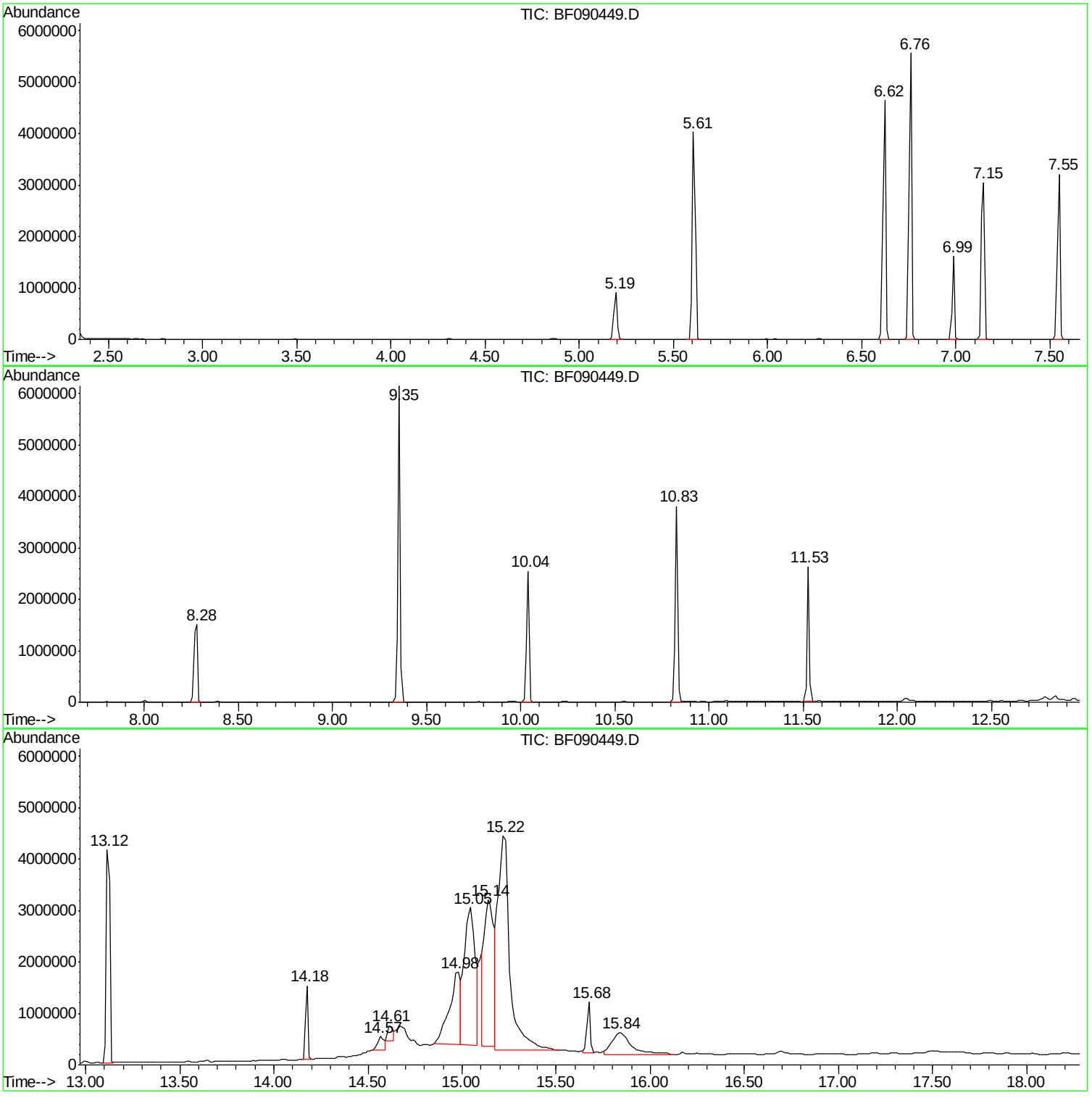
Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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\BF100716\
Data File : BF090449.D
Acq On : 7 Oct 2016 17:16
Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

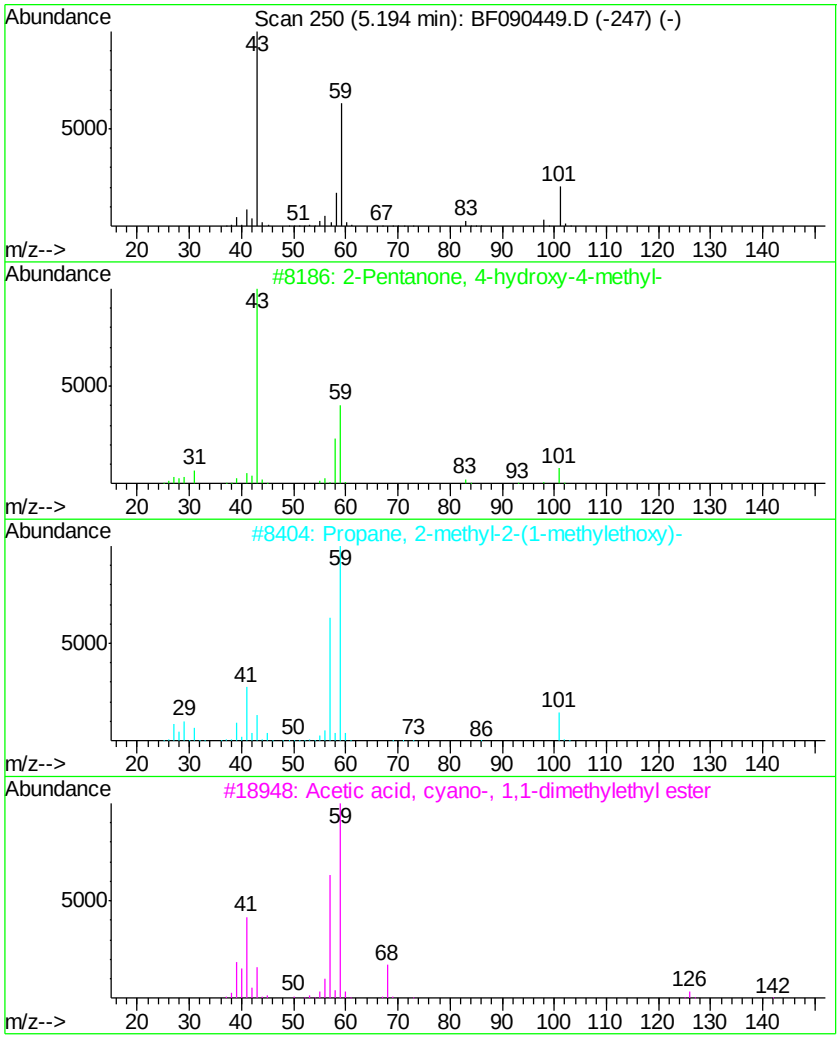
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

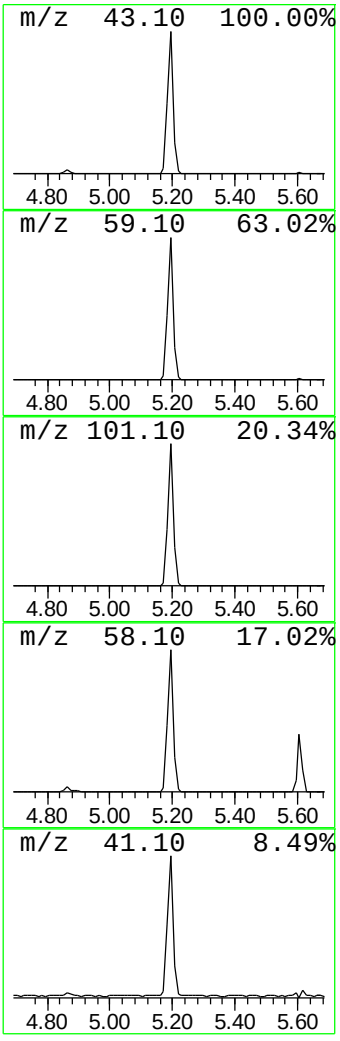
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	14.75 ng	1087480	1,4-Dichlorobenzene-d4	6.99

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	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Guanidine	59	CH5N3	000113-00-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : PB93839BL
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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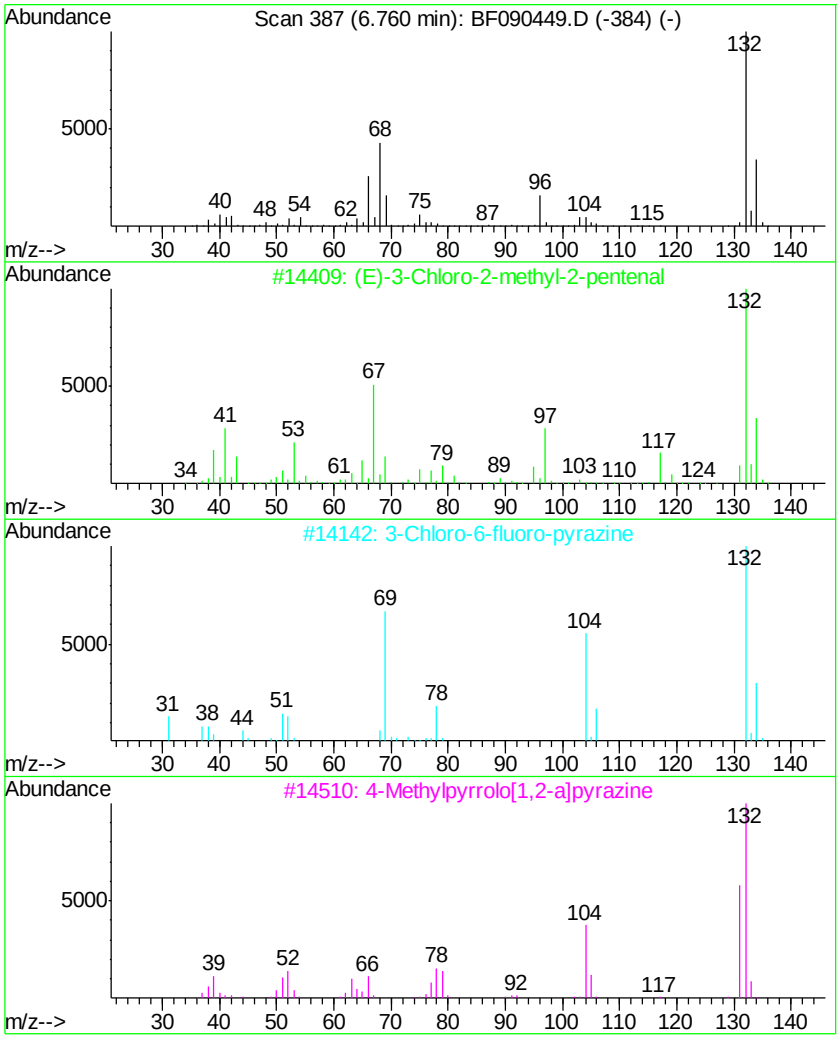
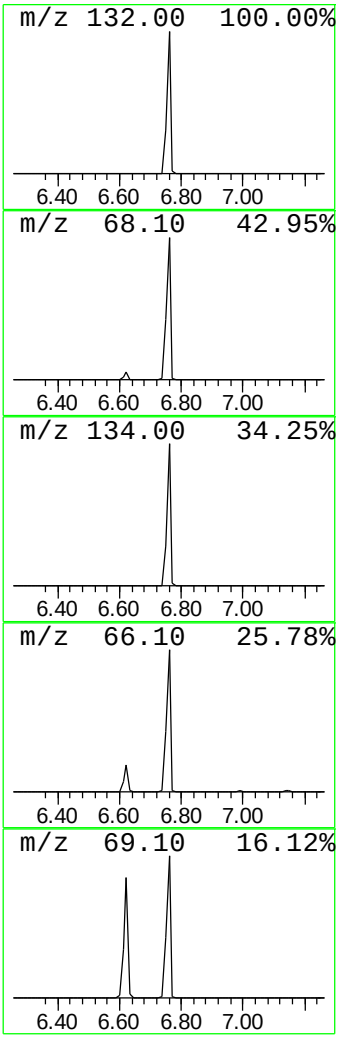
Peak Number 2 unknown6.76 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	71.62 ng	5281090	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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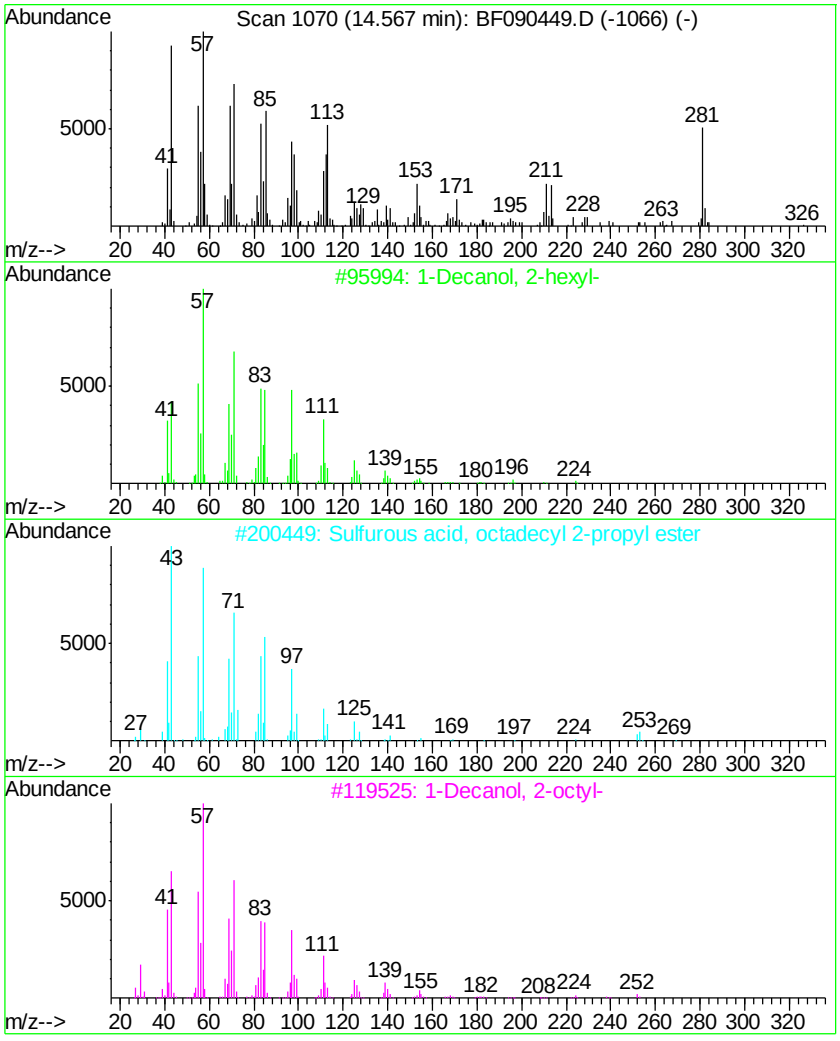
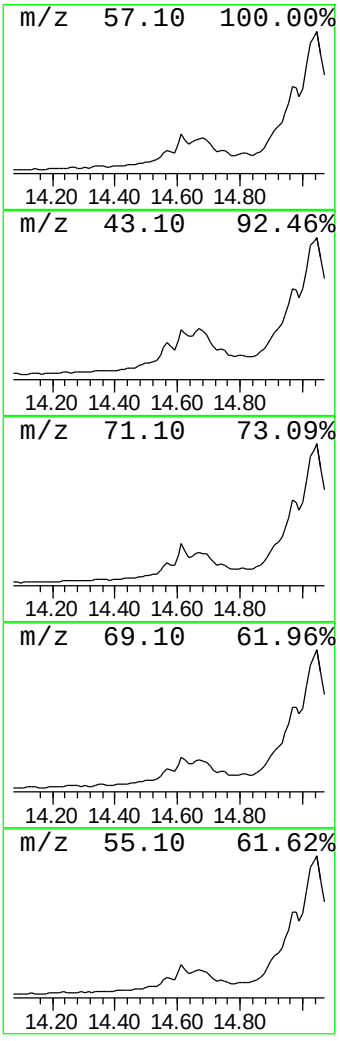
Peak Number 4 unknown14.57 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	8.28 ng	648835	Chrysene-d12	14.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	42
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	38
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	30
4	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	25
5	3-Octadecene, (E)-	252	C18H36	007206-19-1	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090449.D
Acq On : 7 Oct 2016 17:16
Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

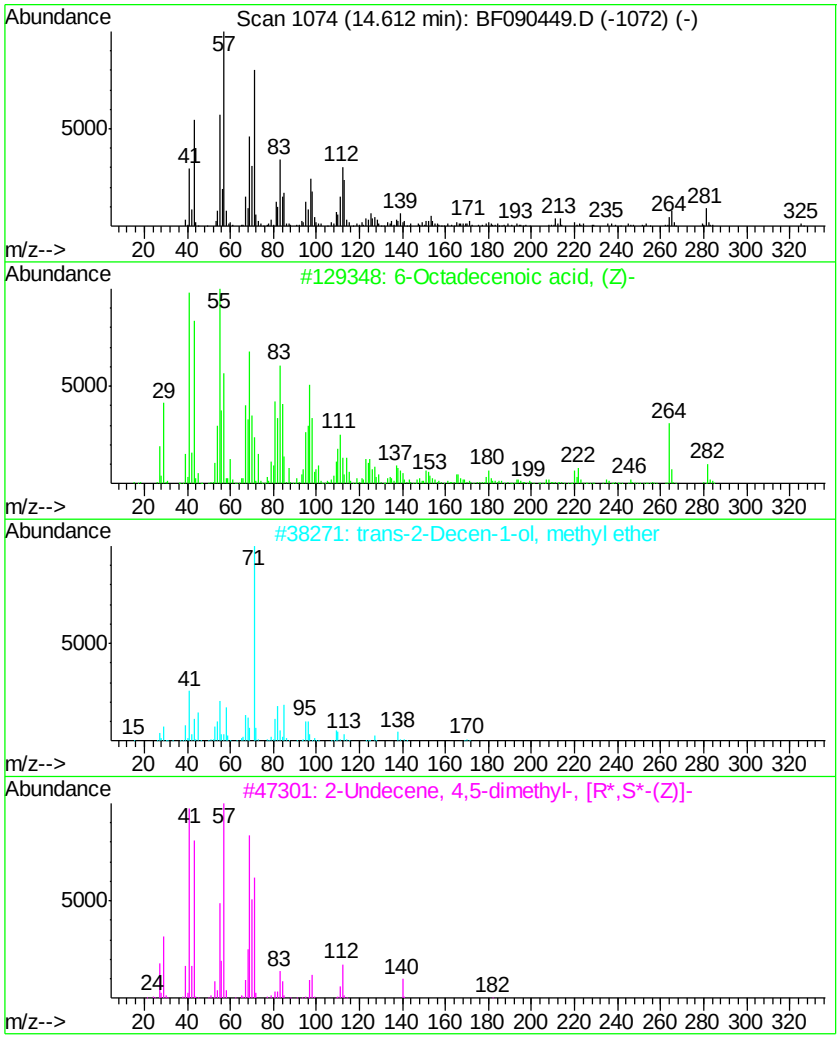
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

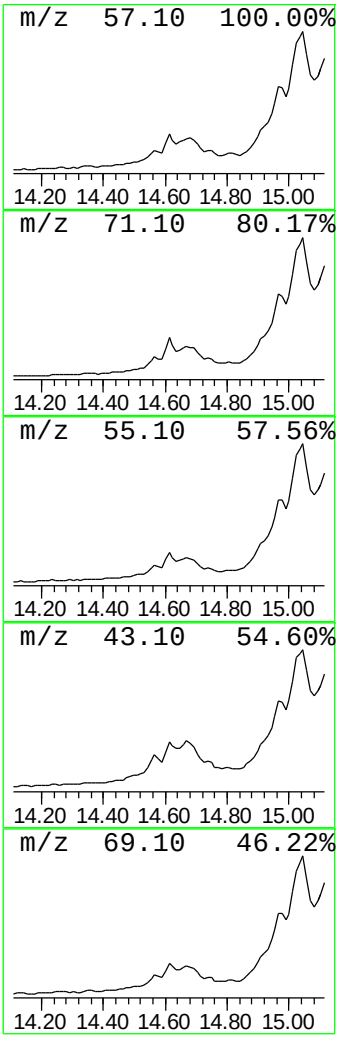
****

Peak Number 5 6-Octadecenoic acid, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	7.65 ng	599452	Chrysene-d12	14.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	56
2	trans-2-Decen-1-ol, methyl ether	170	C11H22O	1000352-66-3	53
3	2-Undecene, 4,5-dimethyl-, [R*,S...	182	C13H26	055170-93-9	52
4	Cyclopropanecarboxamide, N-metha...	139	C8H13NO	1000340-05-6	38
5	2-[Dimethyl(pentafluorophenyl)si...	326	C13H15F5O2Si	1000216-80-8	30





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Acq On : 7 Oct 2016 17:16
Operator : UM/SJ
Sample : PB93839BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

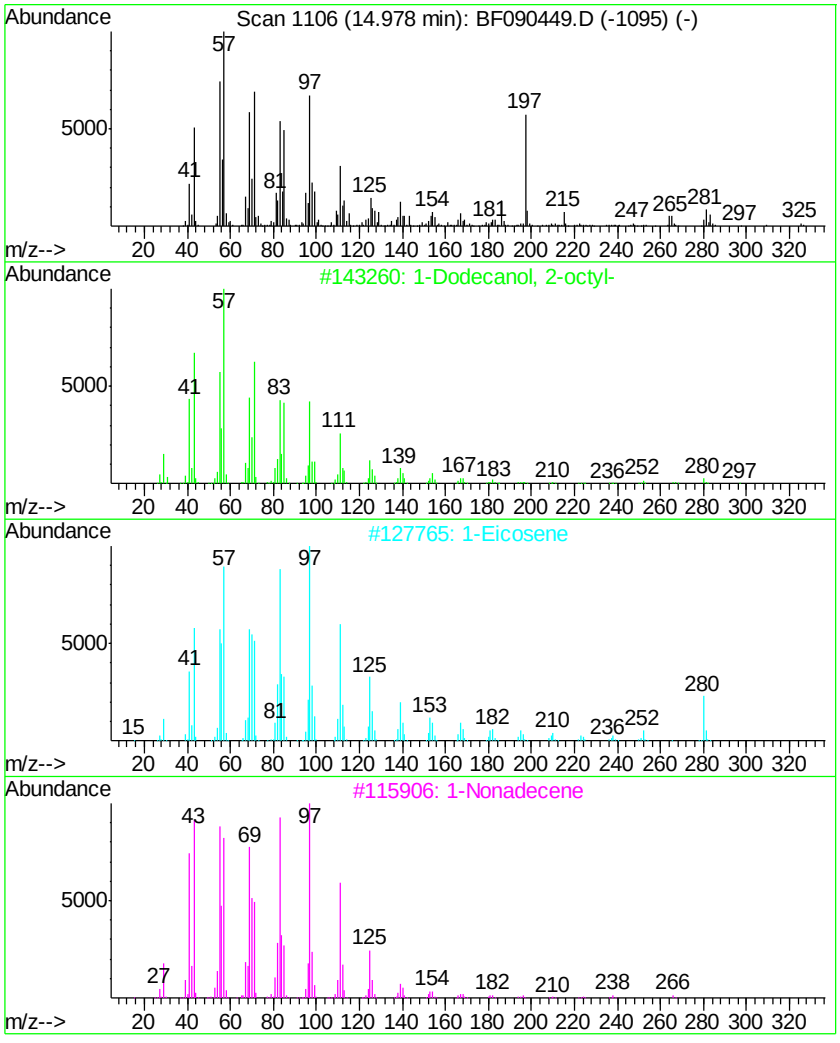
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

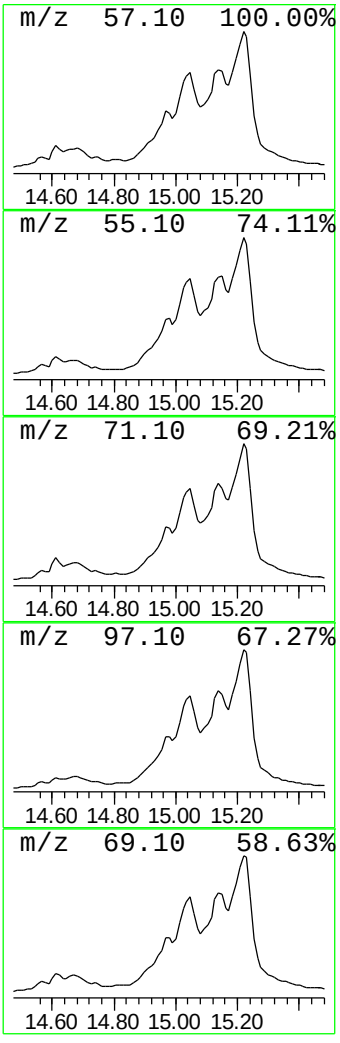
****

Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	91.52 ng	5737100	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	70
2	1-Eicosene	280	C20H40	003452-07-1	64
3	1-Nonadecene	266	C19H38	018435-45-5	64
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	64
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	58





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Instrument : BNA_F
ClientSampleId : PB93839BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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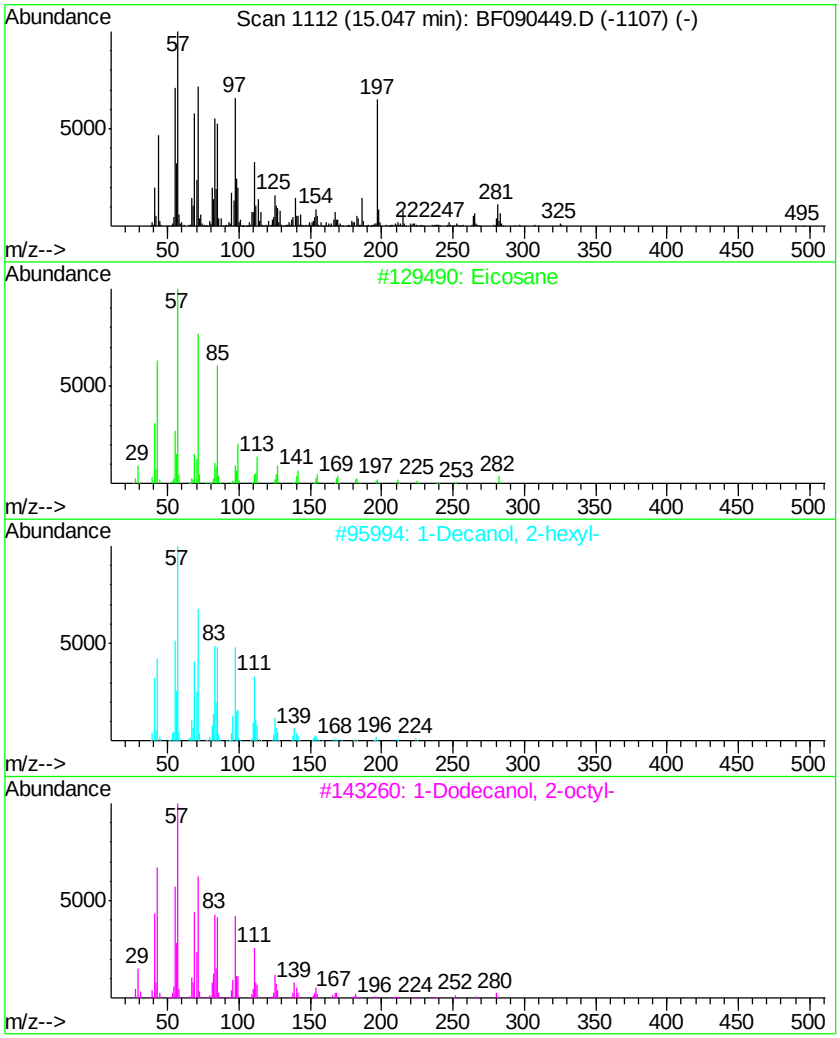
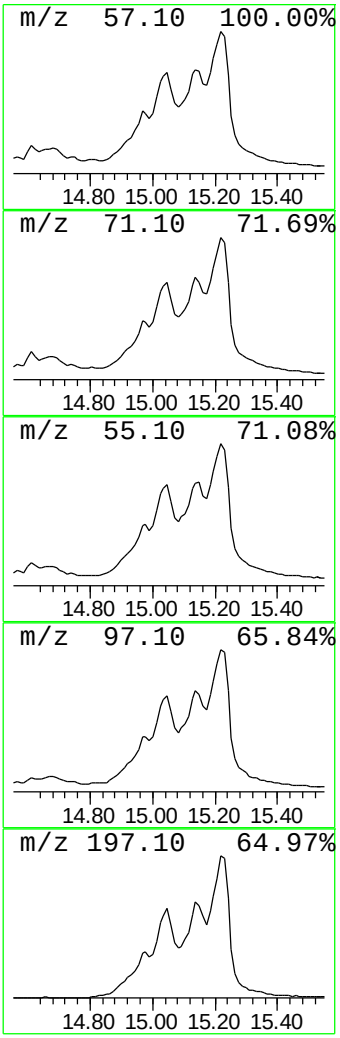
Peak Number 7 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	177.40 ng	11121000	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	70
4	1-Nonadecene	266	C19H38	018435-45-5	64
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	62





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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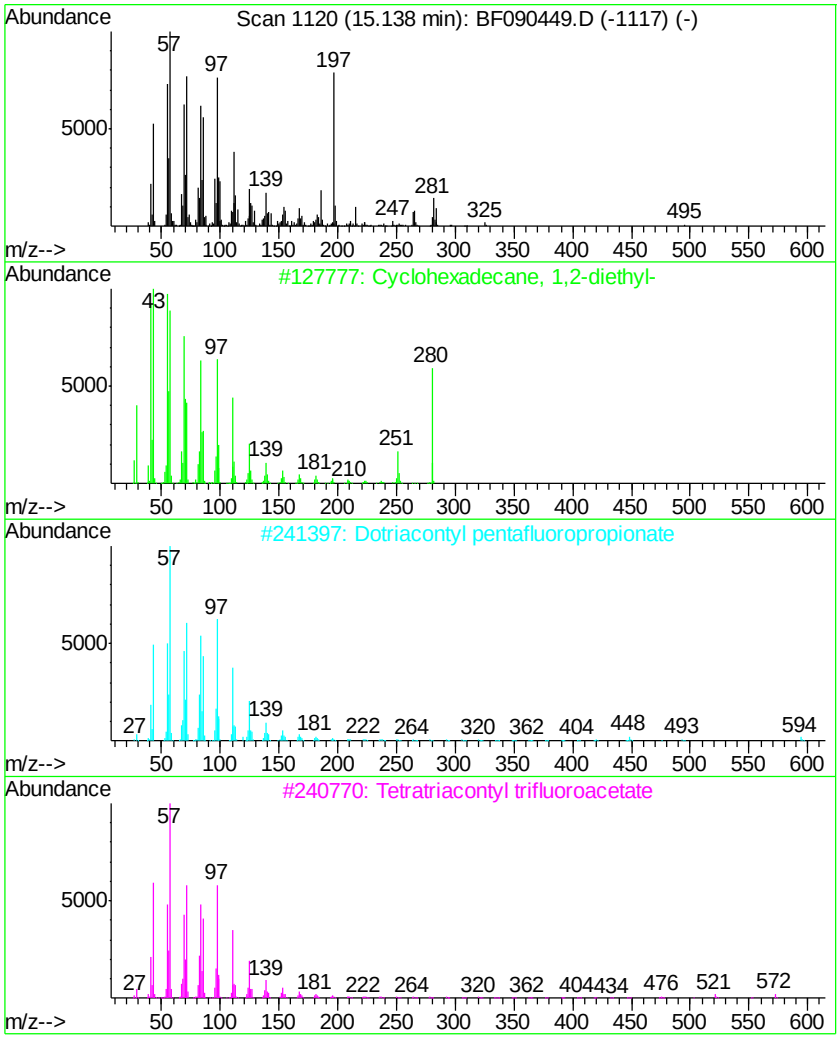
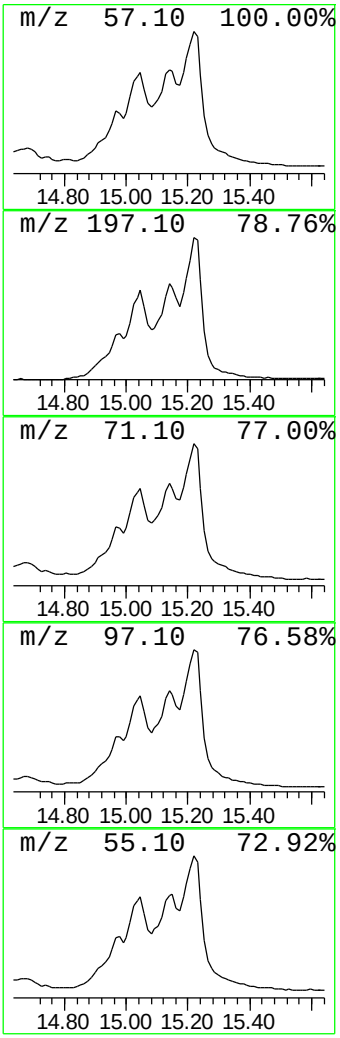
Peak Number 8 Cyclohexadecane, 1,2-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	163.16 ng	10228500	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	66
2	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	62
3	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	62
4	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	62
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	62





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ALS Vial : 13 Sample Multiplier: 1

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

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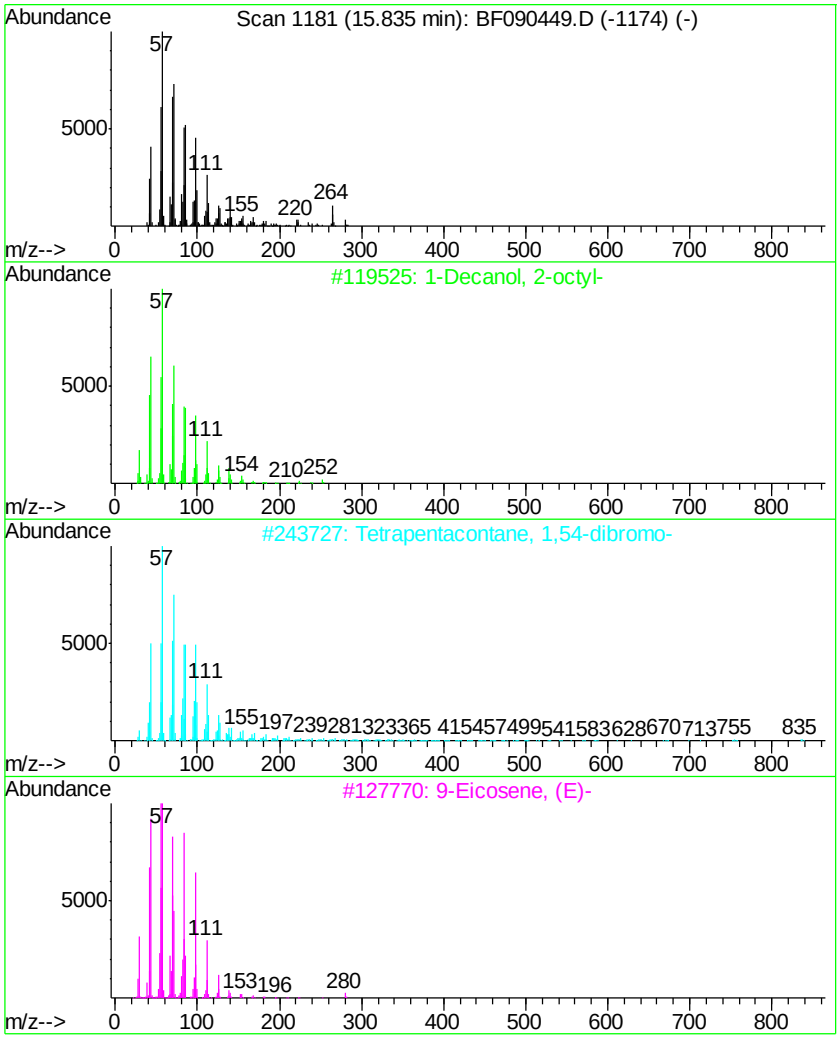
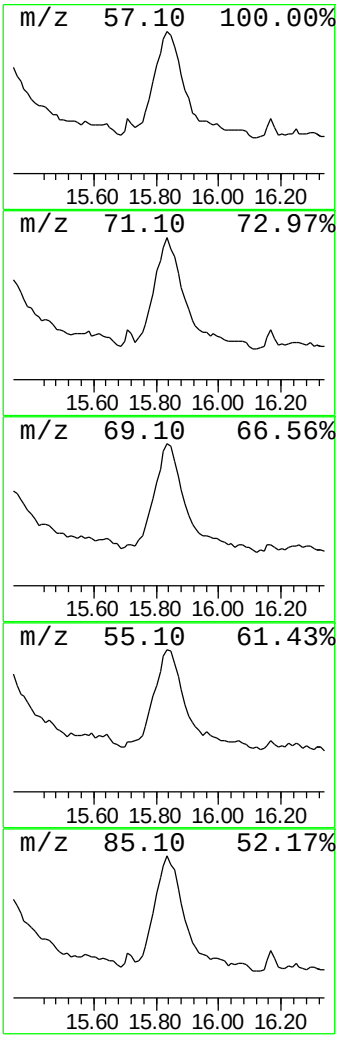
Peak Number 10 1-Decanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	49.92 ng	3129560	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	83
2	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	83
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	83
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
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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...	5.19	14.8	ng	1087480	1	6.99	1474810	20.0
unknown6.76	6.76	71.6	ng	5281090	1	6.99	1474810	20.0
unknown14.57	14.57	8.3	ng	648835	5	14.18	1566980	20.0
6-Octadecenoic ac...	14.61	7.7	ng	599452	5	14.18	1566980	20.0
1-Dodecanol, 2-oc...	14.98	91.5	ng	5737100	6	15.68	1253770	20.0
Eicosane	15.05	177.4	ng	11121000	6	15.68	1253770	20.0
Cyclohexadecane, ...	15.14	163.2	ng	10228500	6	15.68	1253770	20.0
1-Decanol, 2-octyl-	15.84	49.9	ng	3129560	6	15.68	1253770	20.0