LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085078.D
Acq On : 13 Feb 2016 11:27
Operator : SJ/UM
Sample : H1409-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

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-BF021316.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	1.724	10	12	51	rVB	1682504	5449423	100.00%	14.835%
2	3.690	182	184	196	rBV	153747	498029	9.14%	1.356%
3	4.136	220	223	252	rBV	329800	2499181	45.86%	6.804%
4	5.427	333	336	341	rBV	320333	1262727	23.17%	3.438%
5	5.553	345	347	374	rVV	896462	4776223	87.65%	13.002%
6	5.907	374	378	391	rVV2	137910	1108469	20.34%	3.018%
7	6.090	391	394	436	rVB	641726	2991871	54.90%	8.145%
8	6.730	446	450	478	rBV	216252	1948547	35.76%	5.305%
9	7.793	539	543	569	rBV	140611	1045382	19.18%	2.846%
10	9.531	692	695	734	rBV	1024109	3908699	71.73%	10.641%
11	10.228	753	756	765	rBV	57964	278183	5.10%	0.757%
12	10.582	784	787	817	rBV	372587	1346039	24.70%	3.664%
13	11.416	857	860	863	rBV	45648	101265	1.86%	0.276%
14	11.759	885	890	897	rBV	24696	85718	1.57%	0.233%
15	11.885	897	901	925	rVV	483576	2445532	44.88%	6.657%
16	12.194	925	928	938	rVB2	63604	205417	3.77%	0.559%
17	13.005	996	999	1021	rVB	276070	1161029	21.31%	3.161%
18	15.451	1210	1213	1219	rBV2	57962	113766	2.09%	0.310%
19	15.623	1225	1228	1251	rVB	1379678	3187546	58.49%	8.677%
20	16.583	1309	1312	1316	rBV	44401	66683	1.22%	0.182%
21	17.097	1354	1357	1362	rBV	195173	438397	8.04%	1.193%
22	17.177	1362	1364	1377	rVB	365471	849087	15.58%	2.311%
23	18.297	1460	1462	1465	rBV	127268	149403	2.74%	0.407%
24	18.800	1503	1506	1513	rBV	319365	666578	12.23%	1.815%
25	19.326	1549	1552	1560	rVV5	23239	82802	1.52%	0.225%
26	19.737	1582	1588	1592	rBV2	24153	67756	1.24%	0.184%

Sum of corrected areas: 36733752

LSC Report - Integrated Chromatogram

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Misc :
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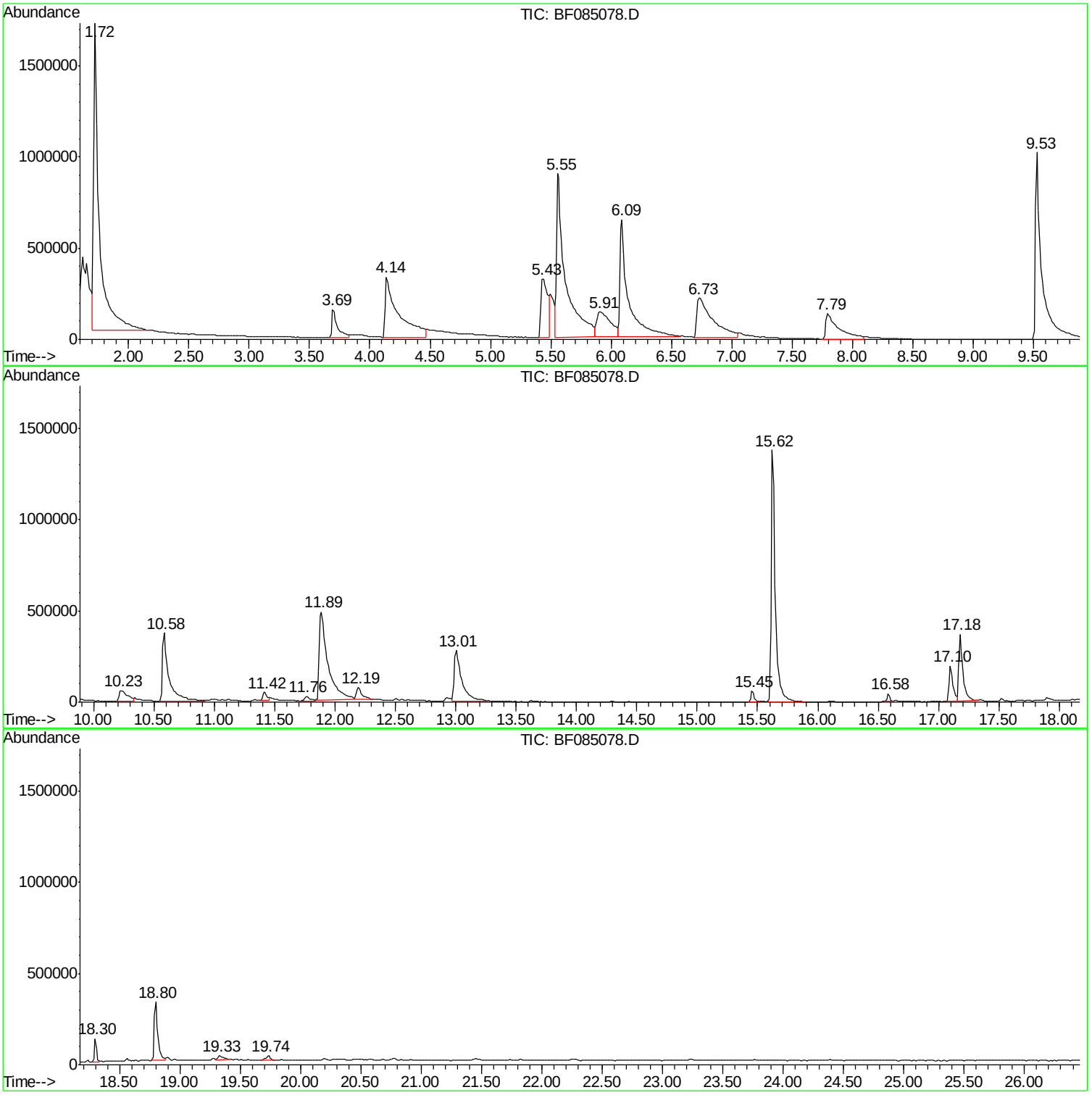
Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.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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Operator : SJ/UM
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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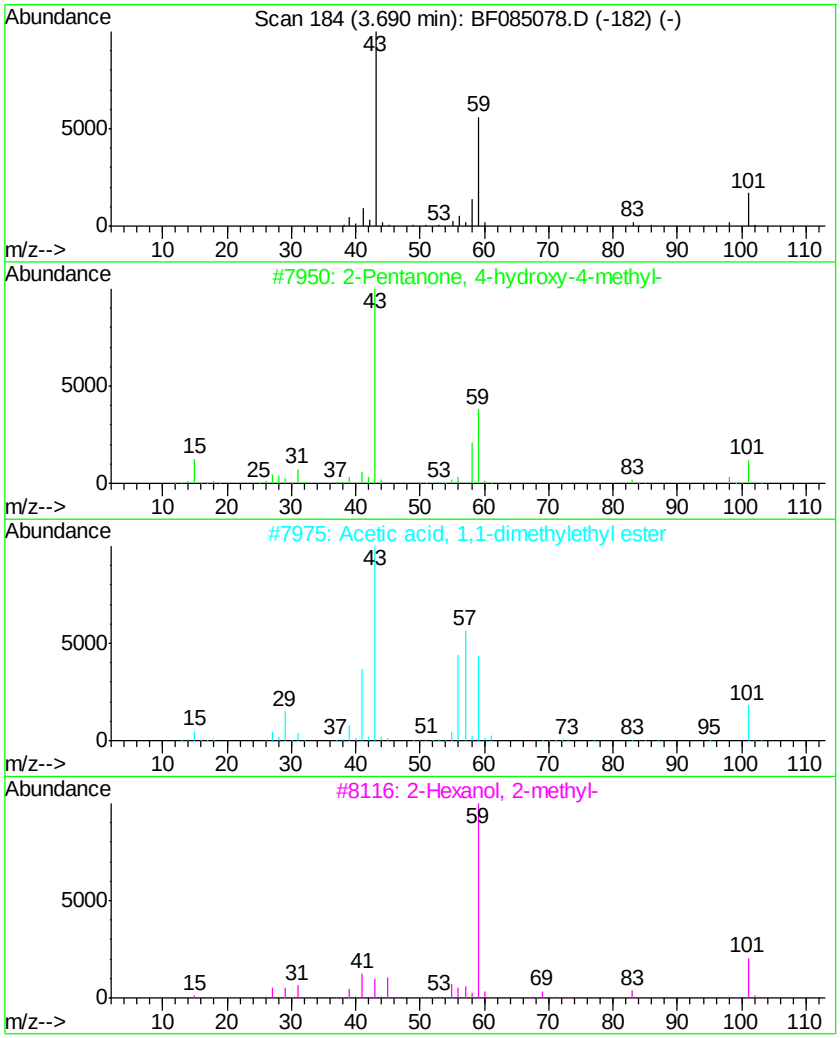
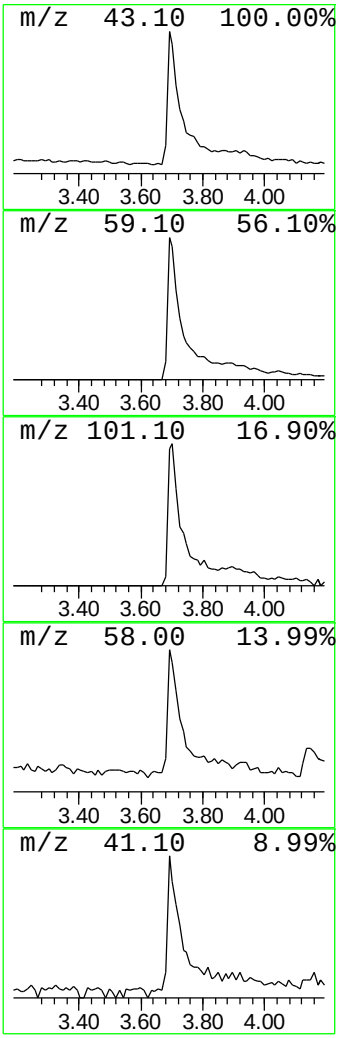
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.69	8.99 ng	498029	1,4-Dichlorobenzene-d4	5.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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Sample : H1409-11
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Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

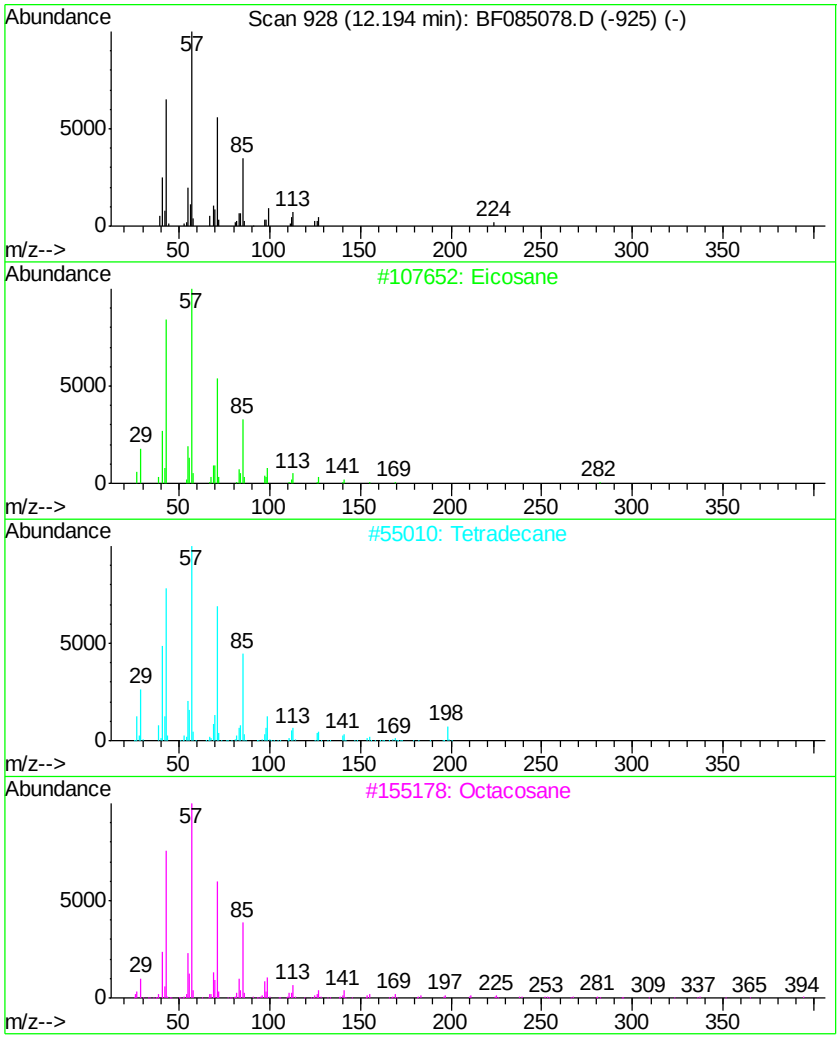
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

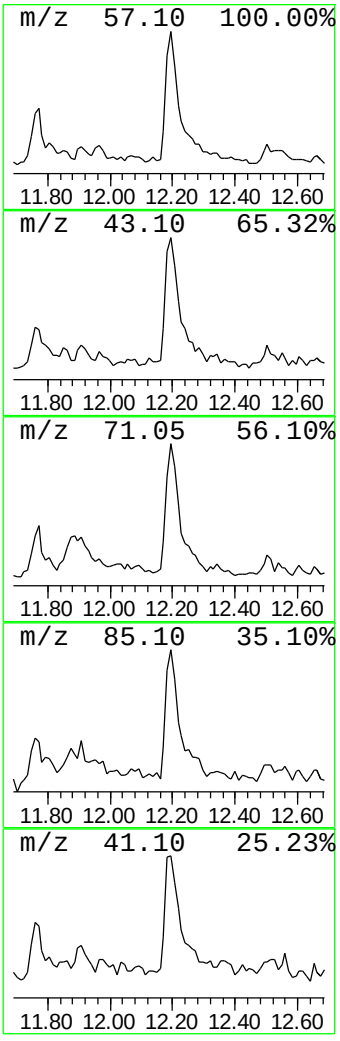
****

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	3.54 ng	205417	Phenanthrene-d10	13.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptacosane	380	C27H56	000593-49-7	86





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Data File : BF085078.D
Acq On : 13 Feb 2016 11:27
Operator : SJ/UM
Sample : H1409-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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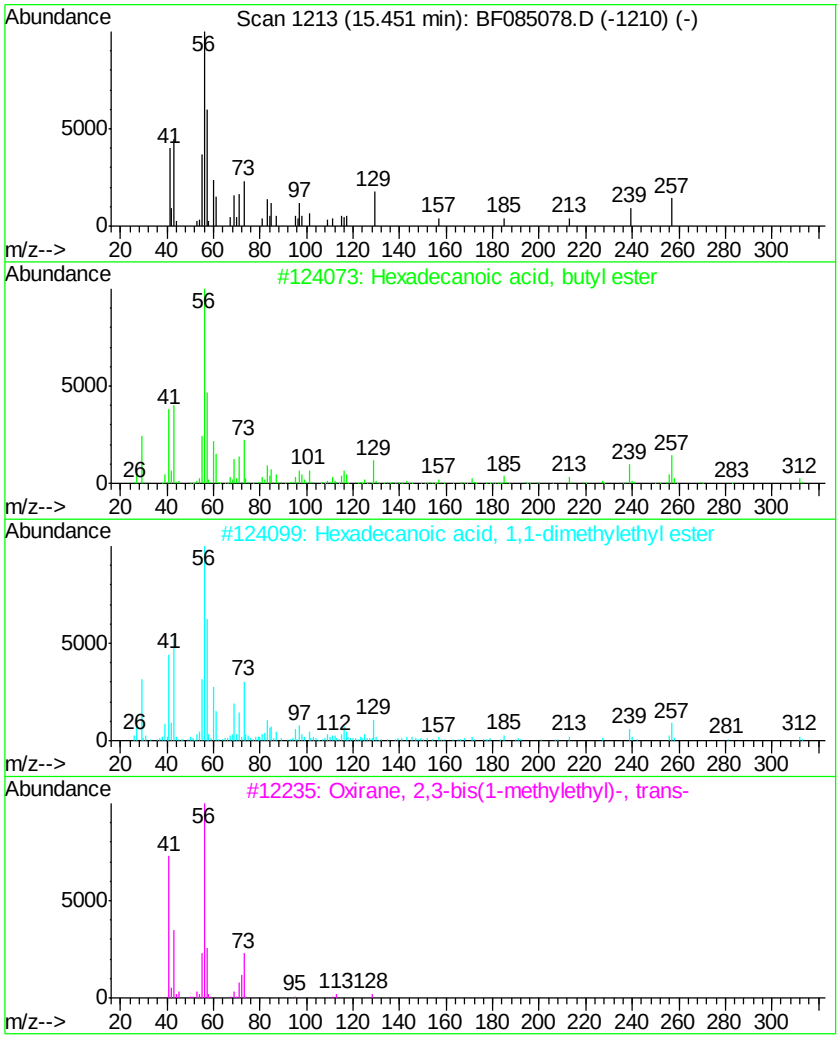
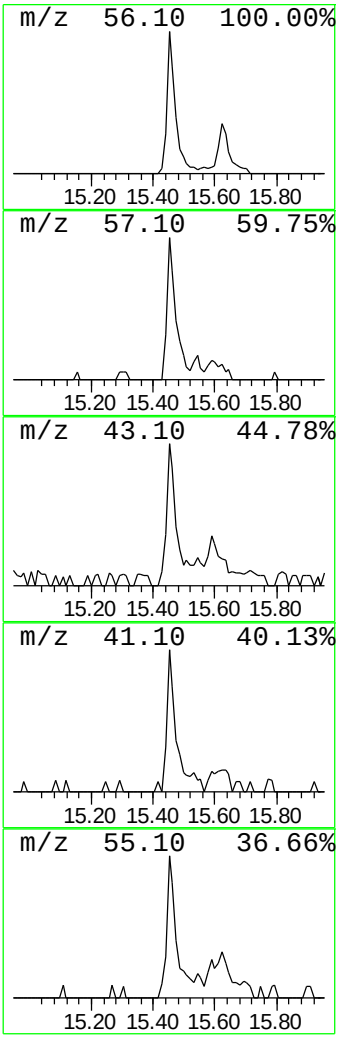
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.68 ng	113766	Chrysene-d12	17.18

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	47
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021416\
Data File : BF085078.D
Acq On : 13 Feb 2016 11:27
Operator : SJ/UM
Sample : H1409-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

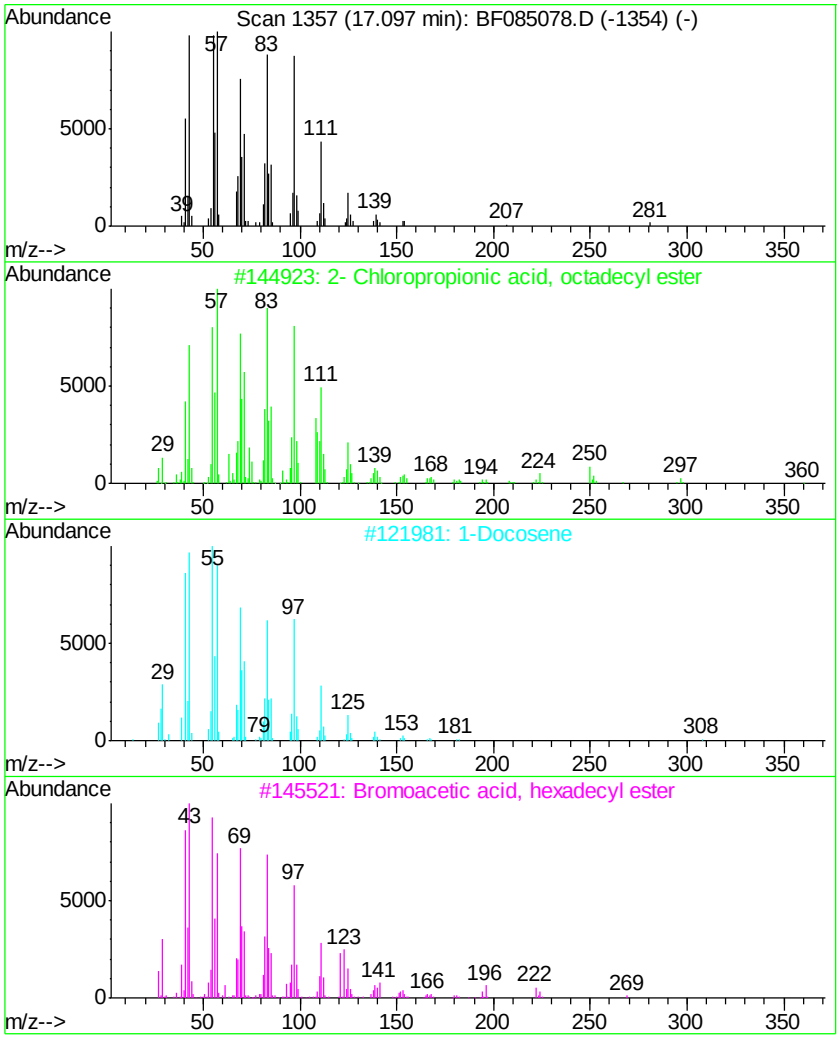
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

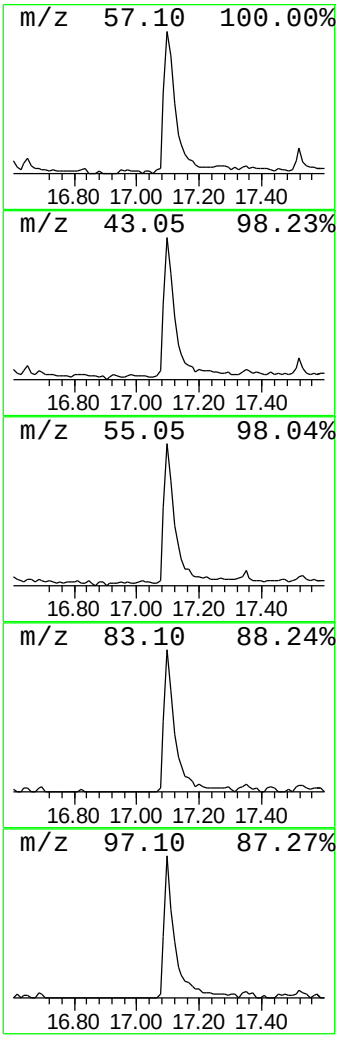
****

Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.10	10.33 ng	438397	Chrysene-d12	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2	1-Docosene	308	C22H44	001599-67-3	89
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87





Library Search Compound Report

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Operator : SJ/UM
Sample : H1409-11
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.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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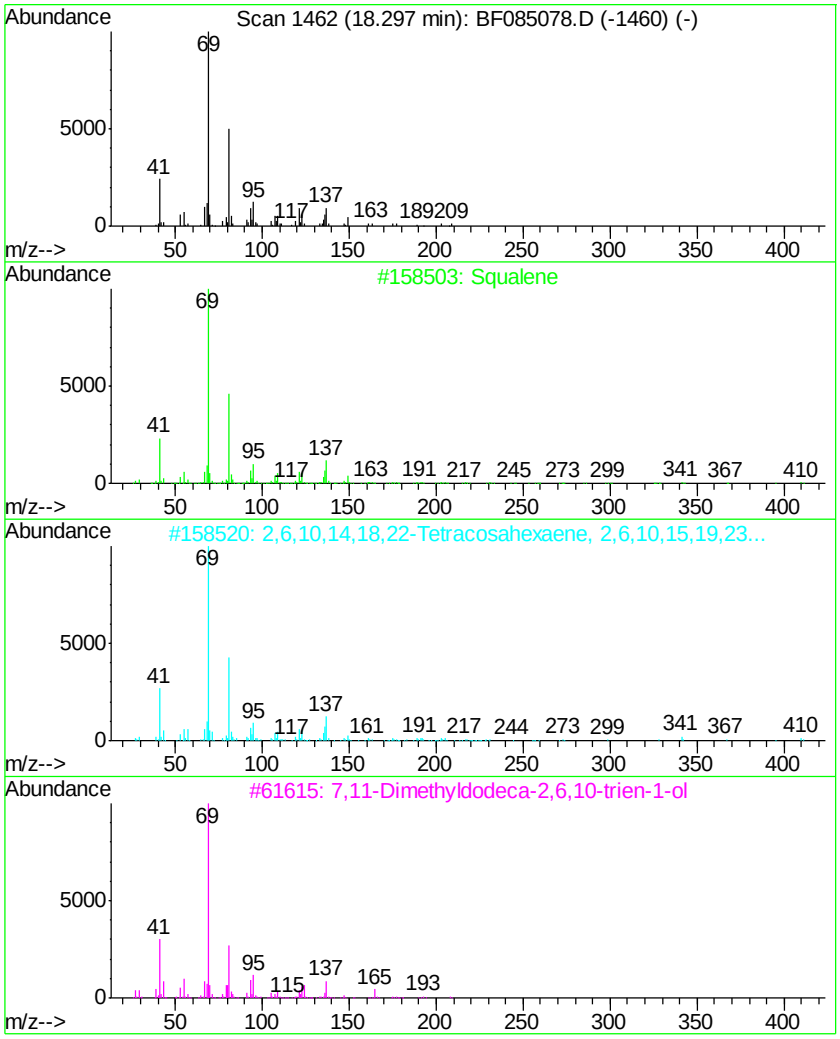
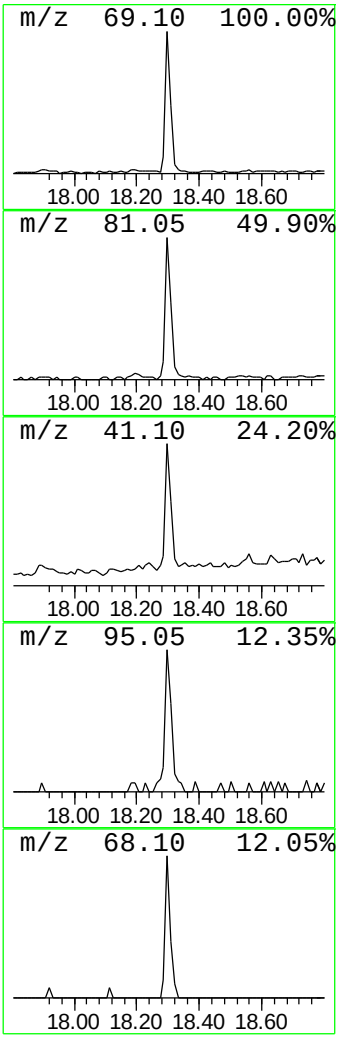
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	4.48 ng	149403	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58





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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B019(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

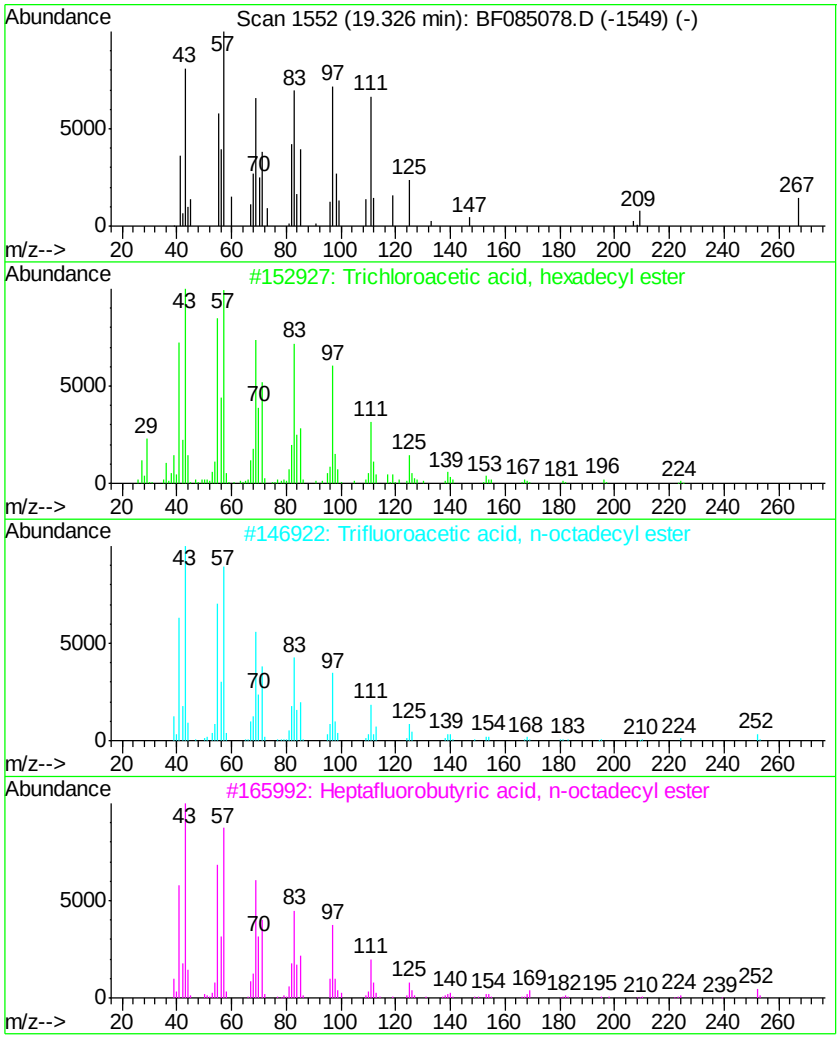
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

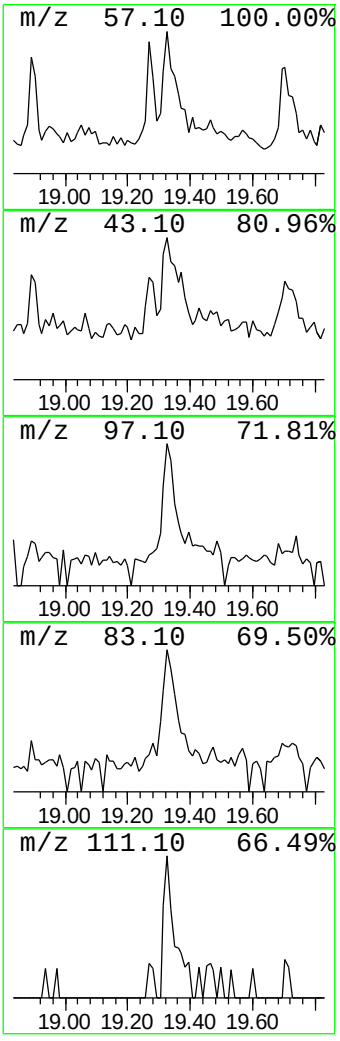
****

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	2.48 ng	82802	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	50
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	47
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	47
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
5	Diallylvinylmethylsilane	152	C9H16Si	119901-87-0	38





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021316.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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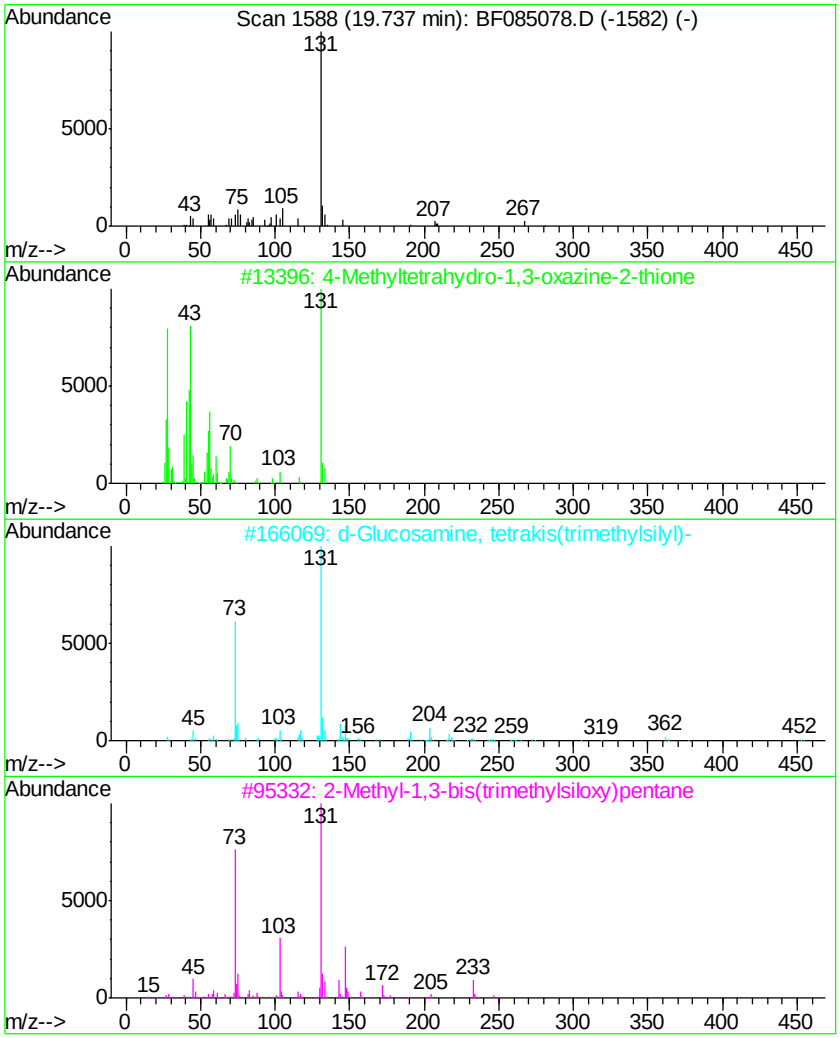
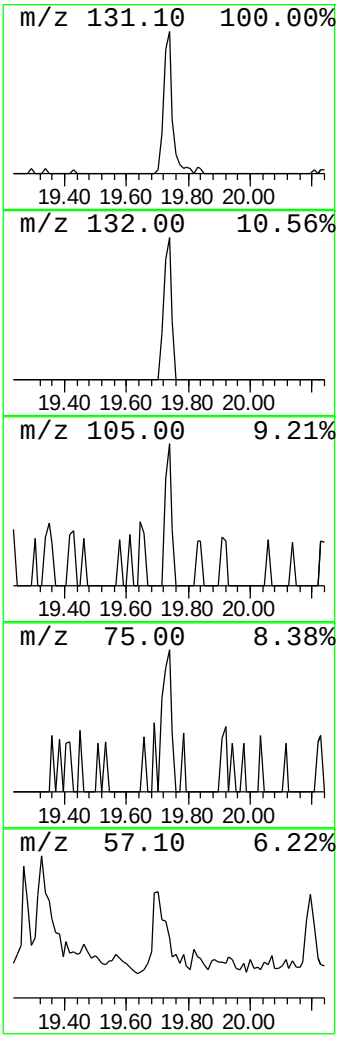
Peak Number 10 4-Methyltetrahydro-1,3-oxaz... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.74	2.03 ng	67756	Perylene-d12	18.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyltetrahydro-1,3-oxazine-2...	131	C5H9NOS	014760-60-2	59
2	d-Glucosamine, tetrakis(trimethy...	467	C18H45NO5Si4	1000079-26-2	38
3	2-Methyl-1,3-bis(trimethylsiloxy...	262	C12H30O2Si2	122424-36-6	36
4	1-Cyclohexyldimethylsilyloxybutane	214	C12H26OSi	1000281-95-6	36
5	trans-2-Ethoxy-.beta.-methyl-.be...	207	C11H13NO3	134040-21-4	16





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.69	9.0	ng	498029	1	5.92	1108470	20.0
Eicosane	12.19	3.5	ng	205417	4	13.01	1161030	20.0
Hexadecanoic acid...	15.45	2.7	ng	113766	5	17.18	849087	20.0
2- Chloropropioni...	17.10	10.3	ng	438397	5	17.18	849087	20.0
Squalene	18.30	4.5	ng	149403	6	18.80	666578	20.0
Trichloroacetic a...	19.33	2.5	ng	82802	6	18.80	666578	20.0
4-Methyltetrahydr...	19.74	2.0	ng	67756	6	18.80	666578	20.0