LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089494.D
Acq On : 1 Aug 2016 4:31
Operator : UM/SJ
Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-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-BF072716.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	1.656	5	6	49	rVB	1027975	2457560	100.00%	19.564%
2	4.582	259	262	271	rBV	232464	447510	18.21%	3.562%
3	5.062	302	304	323	rBV	842178	1156952	47.08%	9.210%
4	6.159	398	400	407	rBV	926794	1134628	46.17%	9.032%
5	6.262	407	409	427	rVB	1187770	1247355	50.76%	9.930%
6	6.490	427	429	440	rVB	202772	230853	9.39%	1.838%
7	6.650	440	443	445	rBV	915074	930887	37.88%	7.410%
8	7.062	477	479	490	rBV	414421	691239	28.13%	5.503%
9	7.782	540	542	544	rBV	239592	252881	10.29%	2.013%
10	8.856	634	636	639	rBV	1031168	1018107	41.43%	8.105%
11	9.256	669	671	674	rBV	197714	185804	7.56%	1.479%
12	9.519	692	694	697	rBV	276504	251783	10.25%	2.004%
13	10.308	761	763	772	rVB	577958	569737	23.18%	4.535%
14	10.445	773	775	778	rBV	25129	27361	1.11%	0.218%
15	10.994	821	823	828	rBV	254208	236231	9.61%	1.881%
16	12.422	946	948	950	rBV	40899	33612	1.37%	0.268%
17	12.582	959	962	964	rBV	793368	1014305	41.27%	8.074%
18	13.485	1039	1041	1046	rBV2	30396	49814	2.03%	0.397%
19	13.611	1050	1052	1055	rBV2	287227	316170	12.87%	2.517%
20	14.262	1107	1109	1111	rBV	39956	35053	1.43%	0.279%
21	14.525	1130	1132	1134	rVV	27324	30111	1.23%	0.240%
22	14.708	1144	1148	1156	rBV2	19411	49385	2.01%	0.393%
23	14.948	1167	1169	1171	rBV	151299	194617	7.92%	1.549%

Sum of corrected areas: 12561955

LSC Report - Integrated Chromatogram

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Operator : UM/SJ
Sample : H4222-10
Misc :
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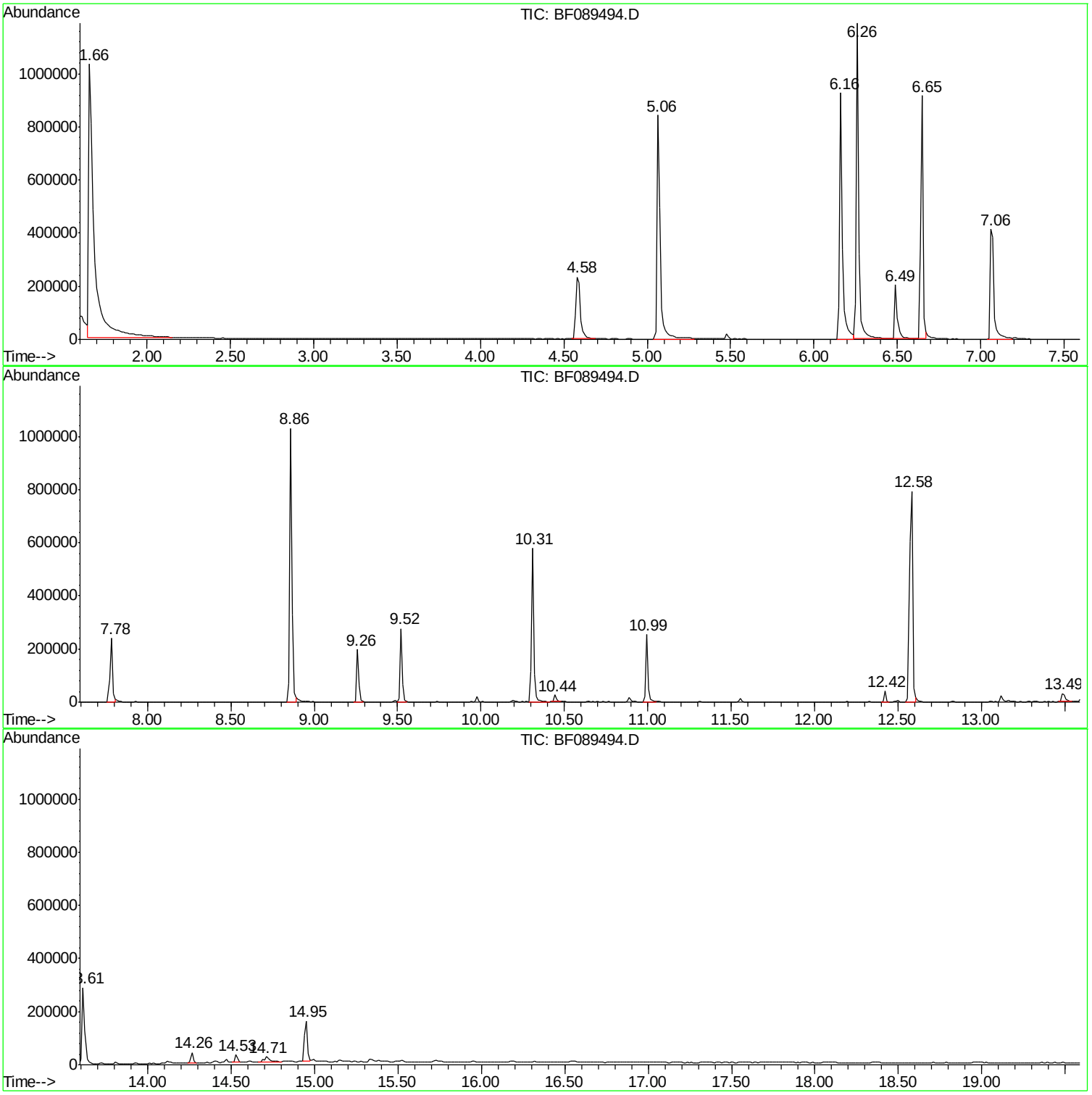
Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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Acq On : 1 Aug 2016 4:31
Operator : UM/SJ
Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

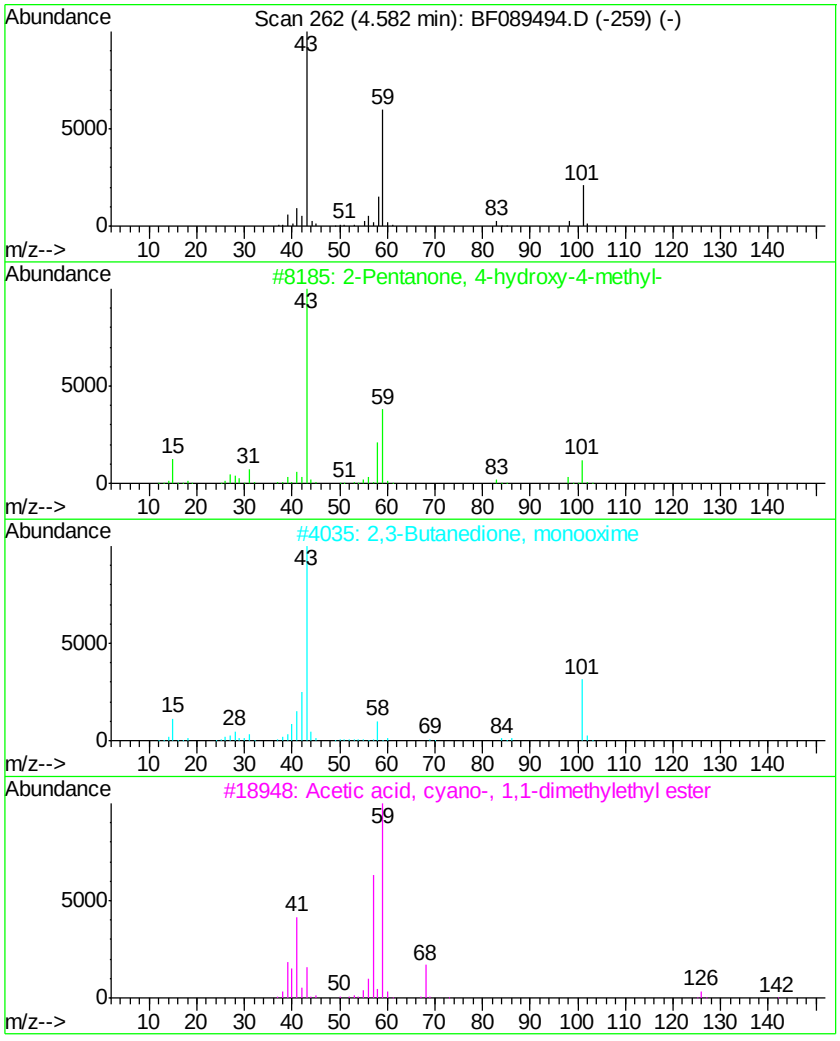
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

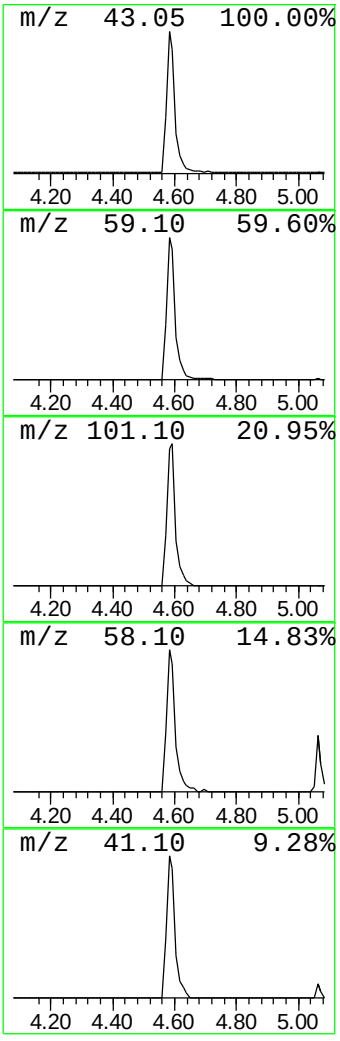
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	38.77 ng	447510	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 1 Aug 2016 4:31
Operator : UM/SJ
Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

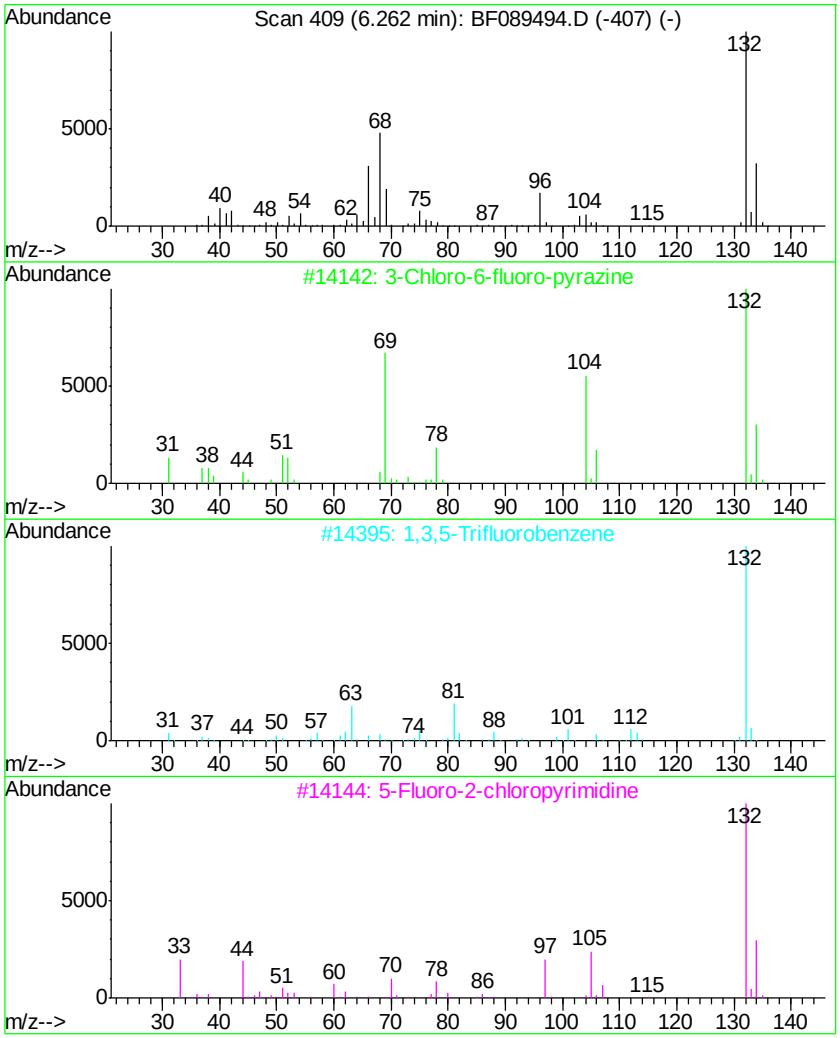
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

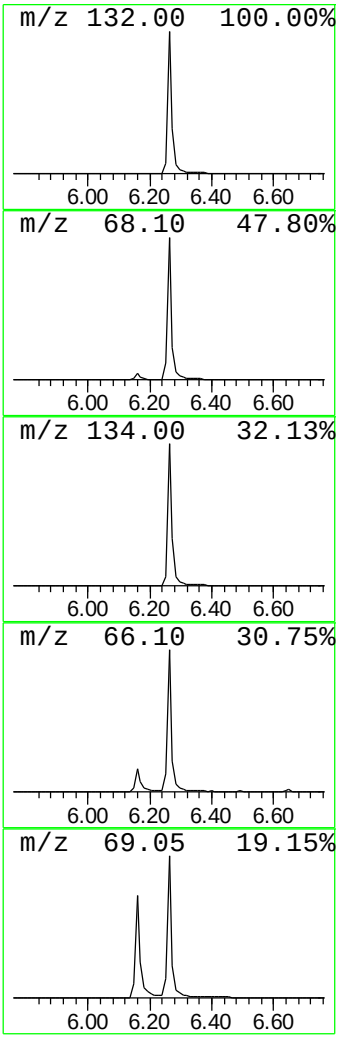
****

Peak Number 3 unknown6.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	108.07 ng	1247360	1,4-Dichlorobenzene-d4	6.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





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Data File : BF089494.D
Acq On : 1 Aug 2016 4:31
Operator : UM/SJ
Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

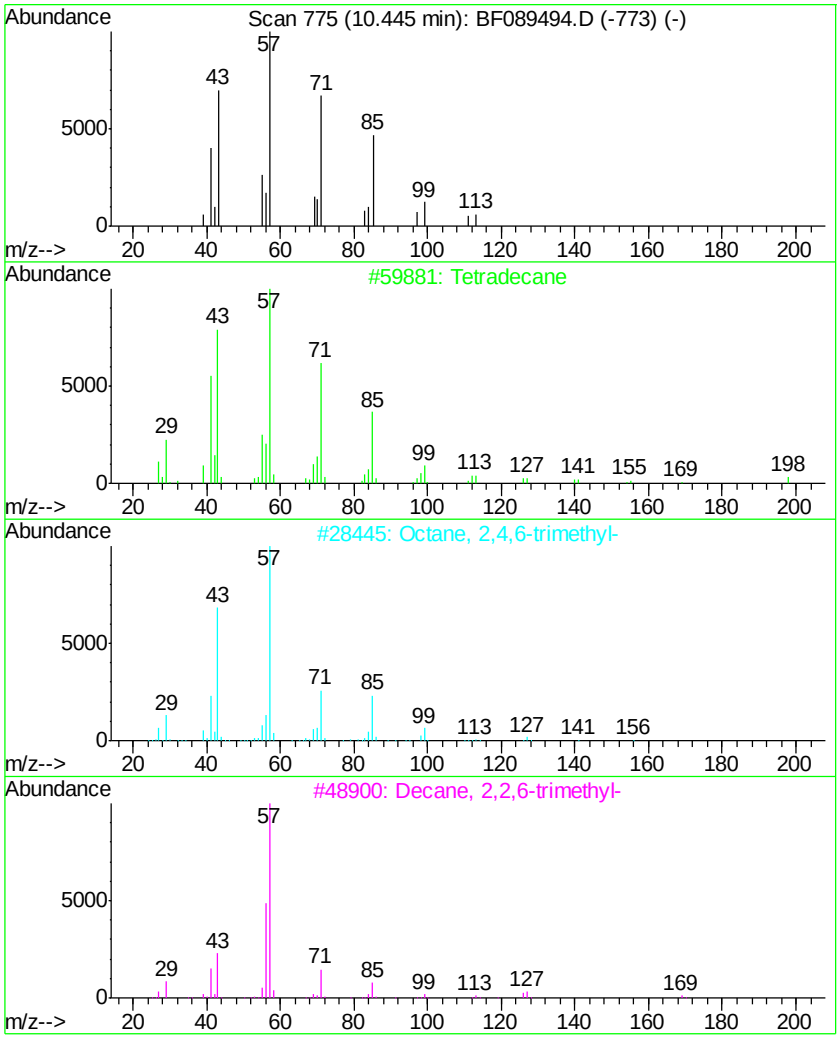
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

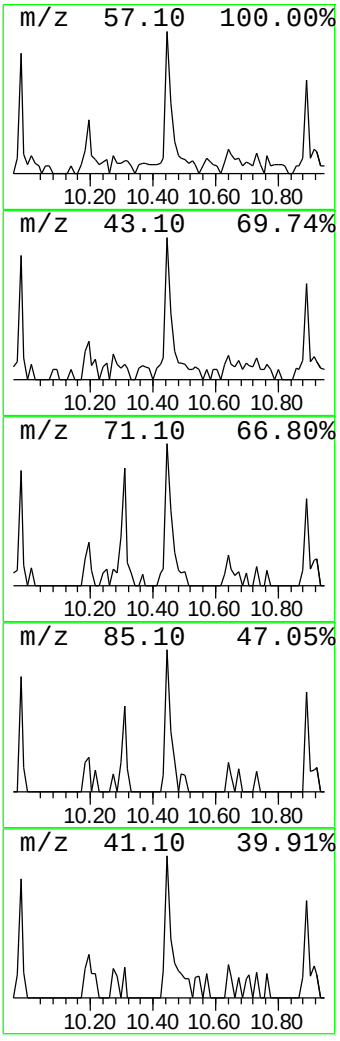
****

Peak Number 5 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.32 ng	27361	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	78
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	78
3	Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64
4	Pentadecane	212	C15H32	000629-62-9	59
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59





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Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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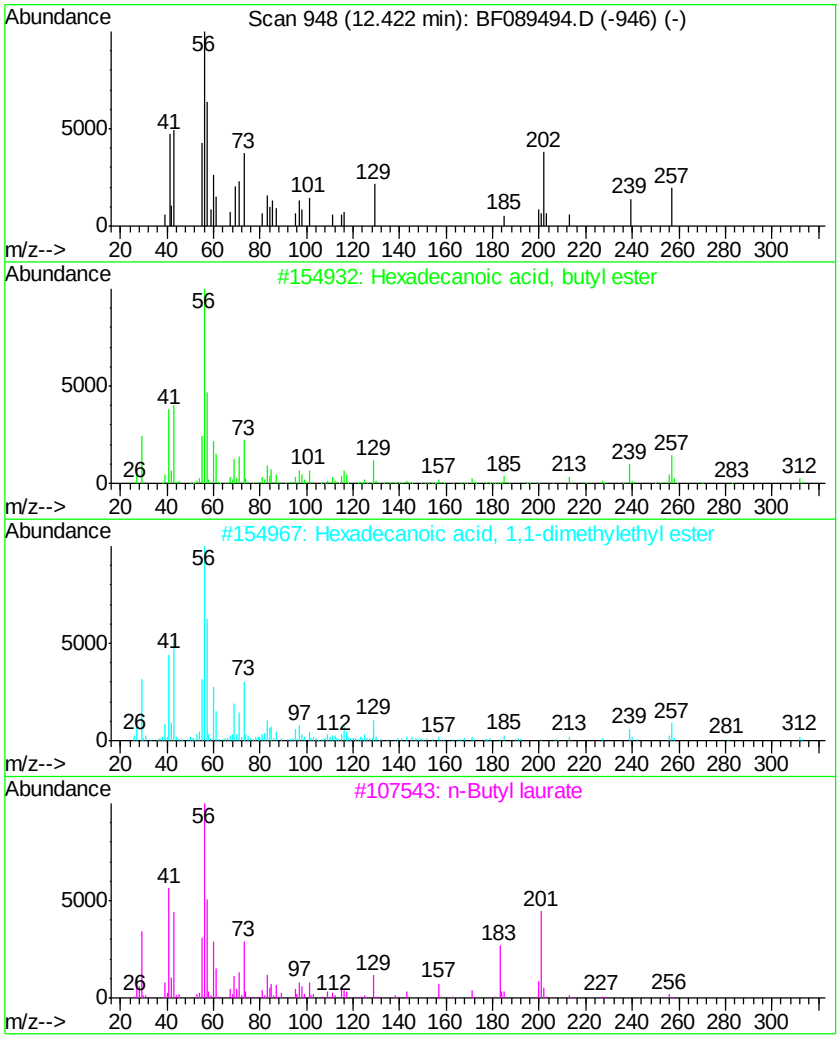
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

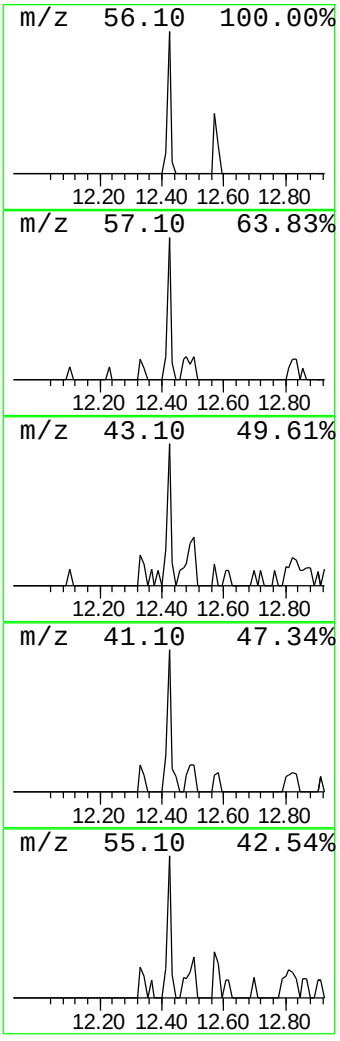
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	2.13 ng	33612	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	n-Butyl laurate	256	C16H32O2	000106-18-3	59
4	Isobutyl laurate	256	C16H32O2	037811-72-6	42
5	Dodecanoic acid tert-butyl ester	256	C16H32O2	007143-18-2	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
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Operator : UM/SJ
Sample : H4222-10
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

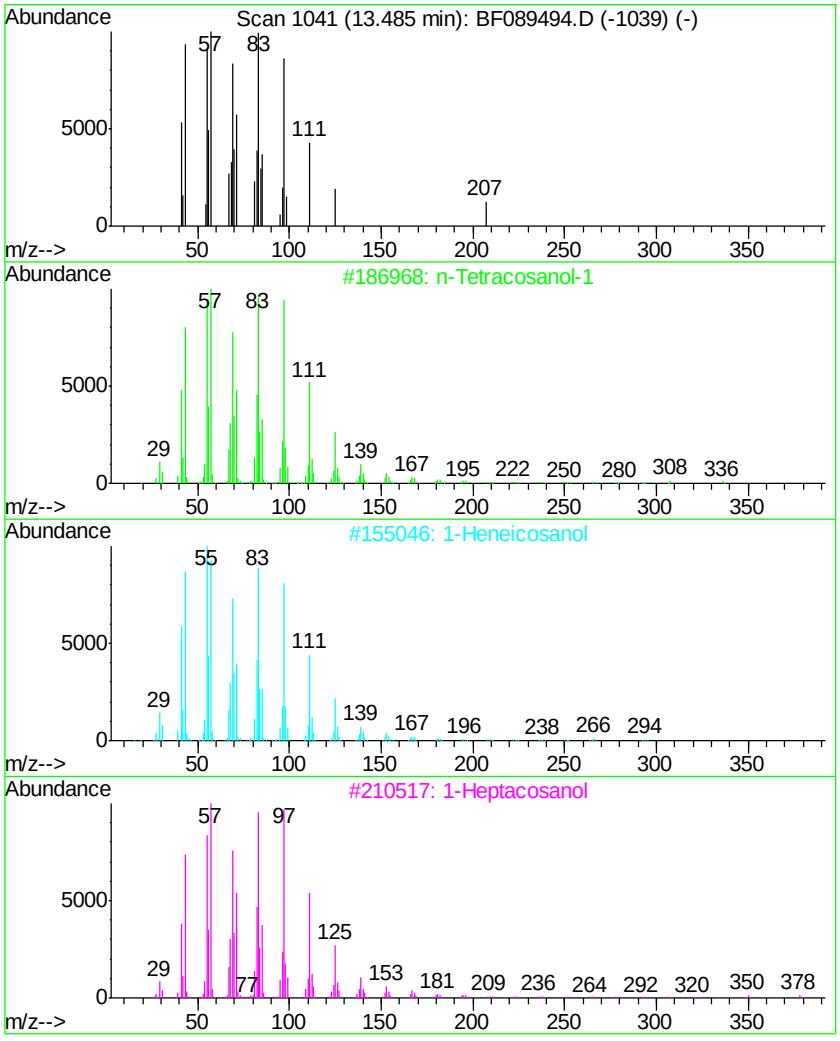
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

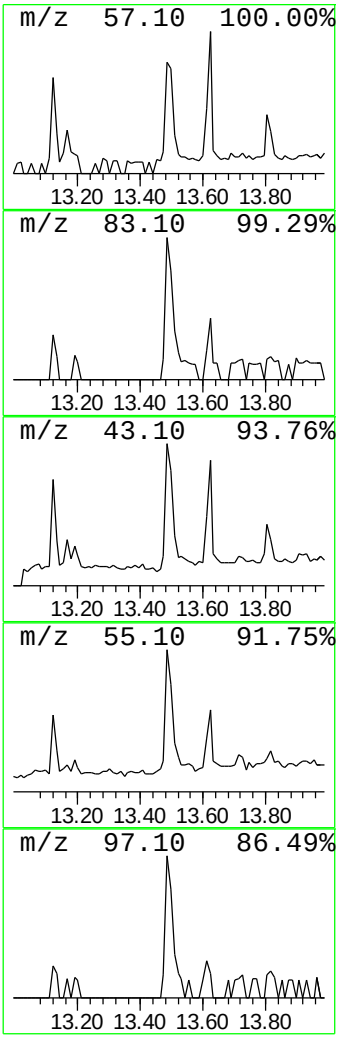
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.15 ng	49814	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Sample : H4222-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-01-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

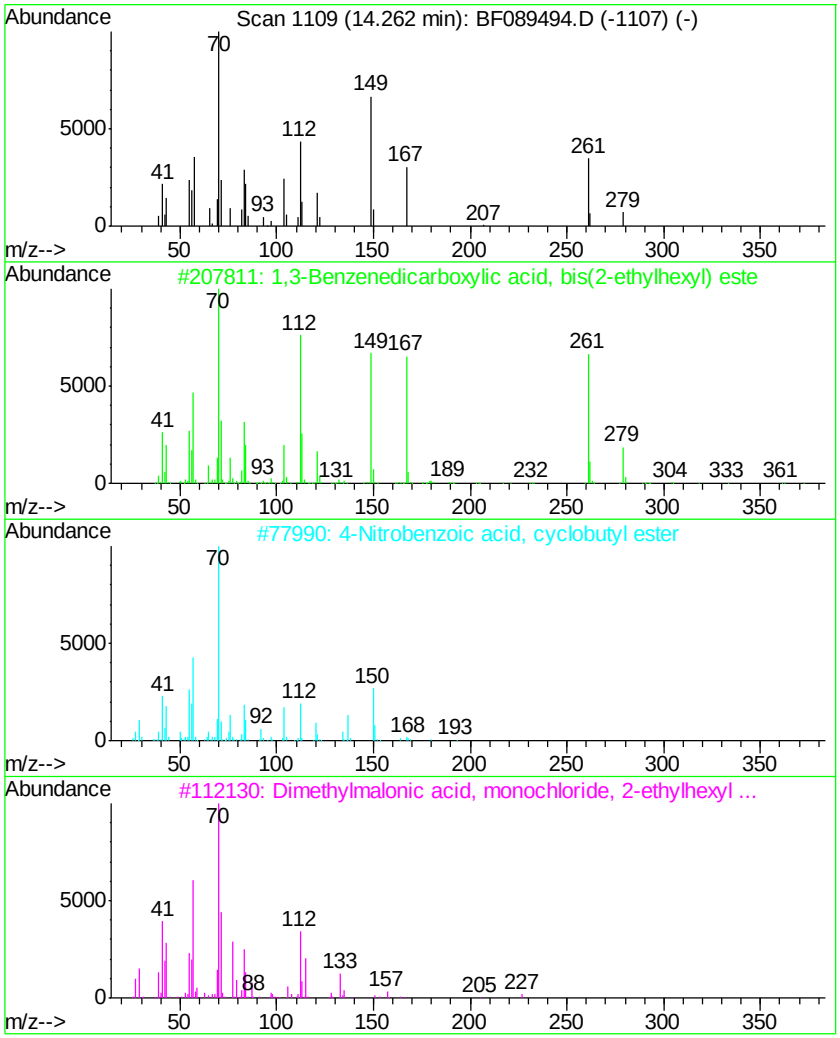
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

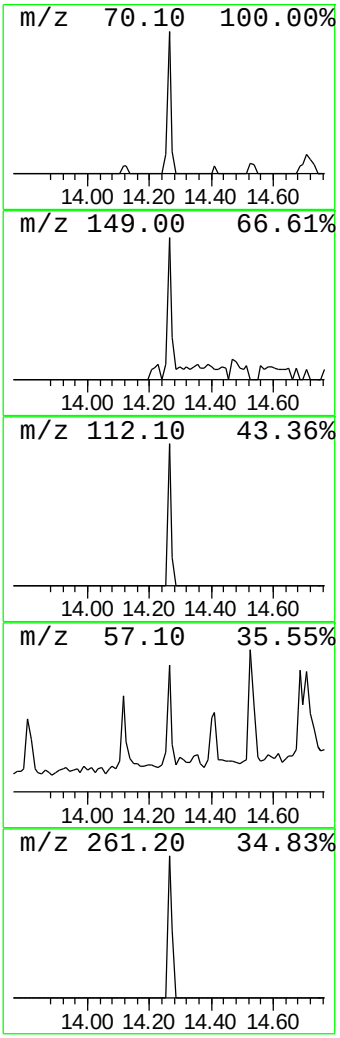
****

Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	2.22 ng	35053	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
2	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	35
3	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	32
4	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
5	Diisooctyl phthalate	390	C24H38O4	000131-20-4	22





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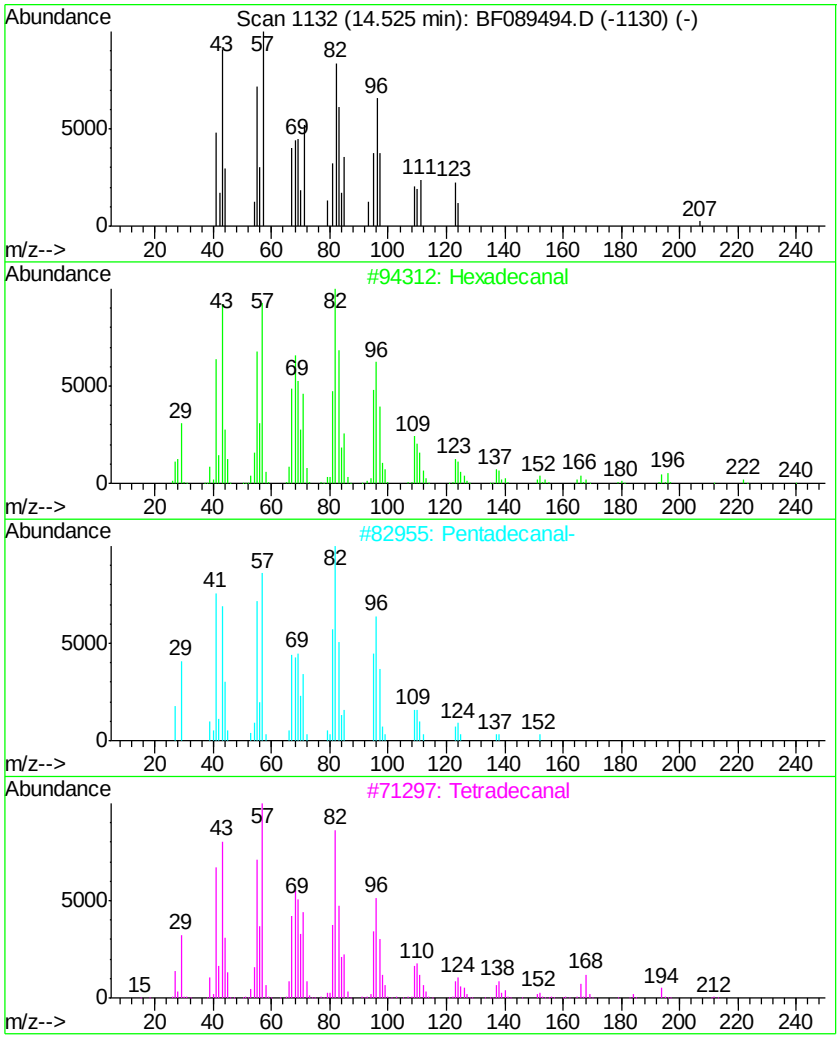
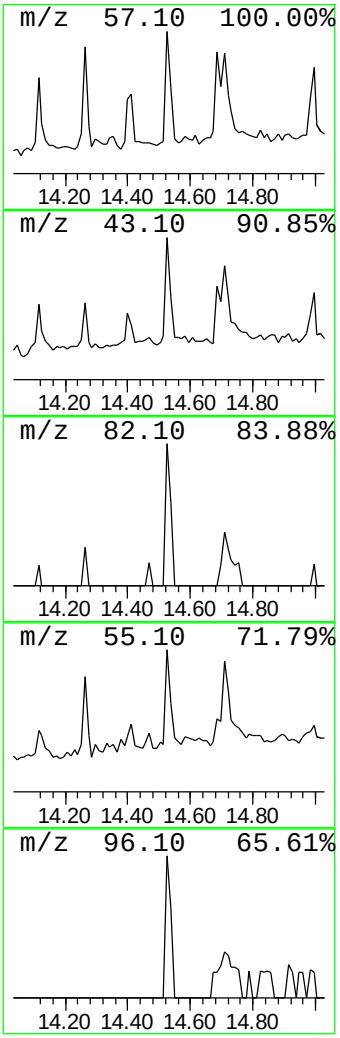
****

Peak Number 9 Hexadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	3.09 ng	30111	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	72
2	Pentadecanal-	226	C15H30O	002765-11-9	68
3	Tetradecanal	212	C14H28O	000124-25-4	64
4	1,19-Eicosadiene	278	C20H38	014811-95-1	64
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
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TIC Library : C:\Database\NIST11.L
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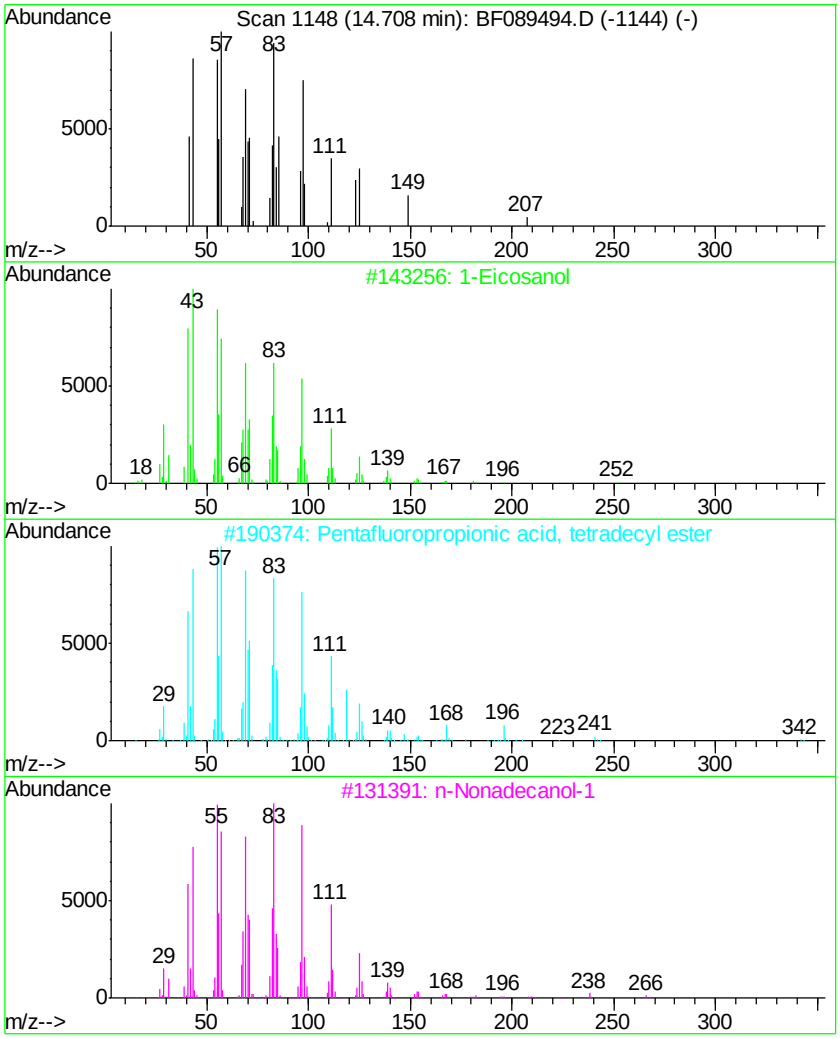
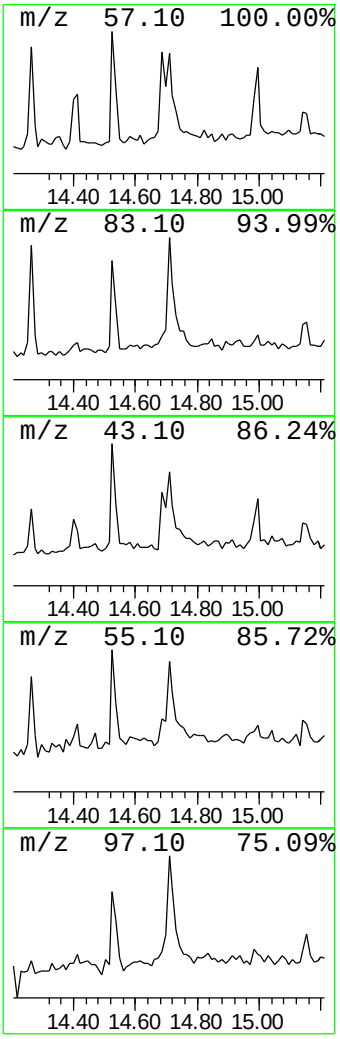
Peak Number 10 1-Eicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.08 ng	49385	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	83
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	81
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	74
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	74
5	n-Pentadecanol	228	C15H32O	000629-76-5	74





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...	4.58	38.8	ng	447510	1	6.49	230853	20.0
unknown6.26	6.26	108.1	ng	1247360	1	6.49	230853	20.0
Tetradecane	10.45	2.3	ng	27361	4	10.99	236231	20.0
Hexadecanoic acid...	12.42	2.1	ng	33612	5	13.61	316170	20.0
n-Tetracosanol-1	13.49	3.1	ng	49814	5	13.61	316170	20.0
1,3-Benzenedicarb...	14.26	2.2	ng	35053	5	13.61	316170	20.0
Hexadecanal	14.53	3.1	ng	30111	6	14.95	194617	20.0
1-Eicosanol	14.71	5.1	ng	49385	6	14.95	194617	20.0