LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102606.D
Acq On : 29 Jan 2018 19:28
Operator : SJ/JU
Sample : J1344-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-3-WW(5-6)

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-BF012218.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	4.928	479	483	494	rBV	90400	134516	2.82%	0.327%
2	5.334	547	552	555	rBV	4158822	4223490	88.53%	10.272%
3	6.369	722	728	744	rBV	3821890	4625506	96.96%	11.249%
4	6.487	744	748	751	rBV	4277818	4395820	92.15%	10.691%
5	6.710	783	786	796	rBV	1143390	1064754	22.32%	2.590%
6	6.869	809	813	816	rBV	3714837	3393857	71.14%	8.254%
7	7.286	879	884	896	rBV	2866428	3033700	63.59%	7.378%
8	7.998	1001	1005	1026	rVB	1505174	1539354	32.27%	3.744%
9	9.075	1182	1188	1191	rBV	4858694	4770499	100.00%	11.602%
10	9.469	1251	1255	1264	rBV	772861	739027	15.49%	1.797%
11	9.751	1298	1303	1316	rVB	1801612	1680393	35.22%	4.087%
12	10.175	1372	1375	1377	rVB2	106461	82455	1.73%	0.201%
13	10.545	1434	1438	1452	rBV	2545617	2676093	56.10%	6.508%
14	10.645	1452	1455	1462	rVB	106418	113317	2.38%	0.276%
15	11.239	1552	1556	1565	rBV	1550139	1544018	32.37%	3.755%
16	12.827	1820	1826	1829	rBV	3824866	4096148	85.86%	9.962%
17	13.715	1973	1977	1986	rBV	311395	445656	9.34%	1.084%
18	13.880	2001	2005	2013	rBV	1227569	1240545	26.00%	3.017%
19	13.962	2017	2019	2021	rBV2	61692	50309	1.05%	0.122%
20	14.615	2127	2130	2136	rBV	202922	250411	5.25%	0.609%
21	15.309	2243	2248	2258	rBV	772878	1018261	21.34%	2.476%

Sum of corrected areas: 41118129

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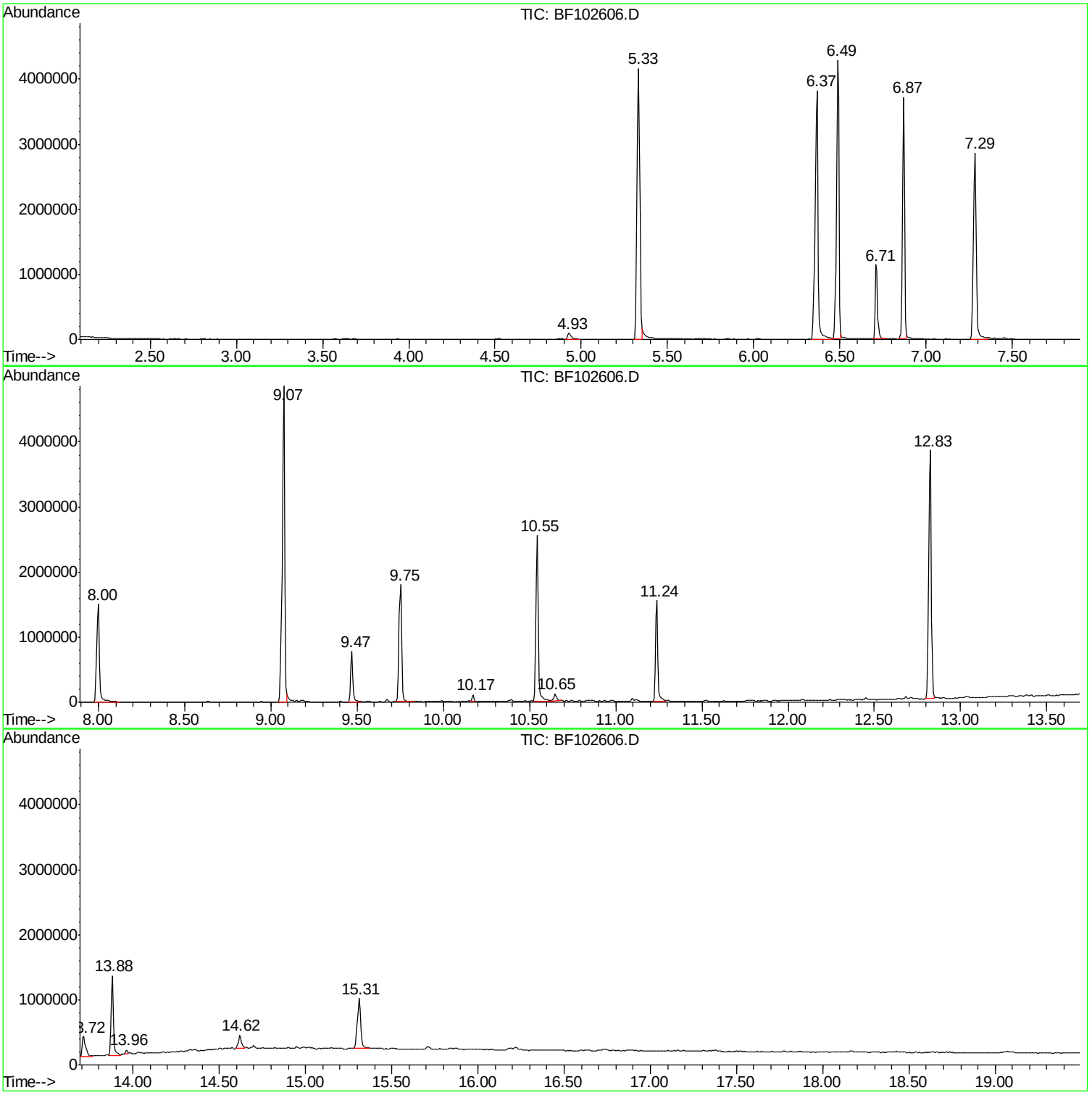
BNA_F
ClientSampleId :
8-SAN-3-WW(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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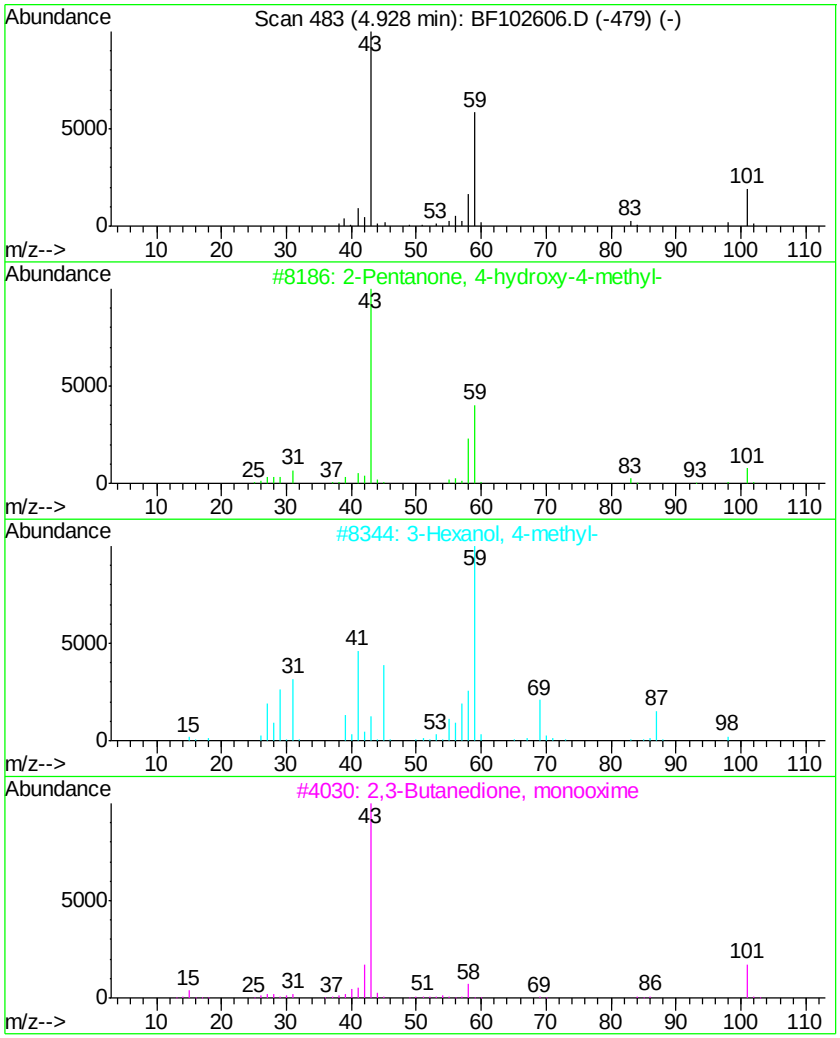
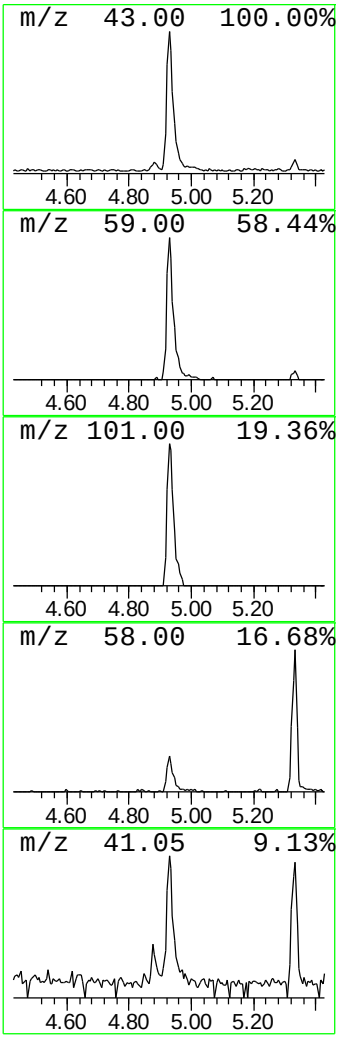
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.53 ng	134516	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9





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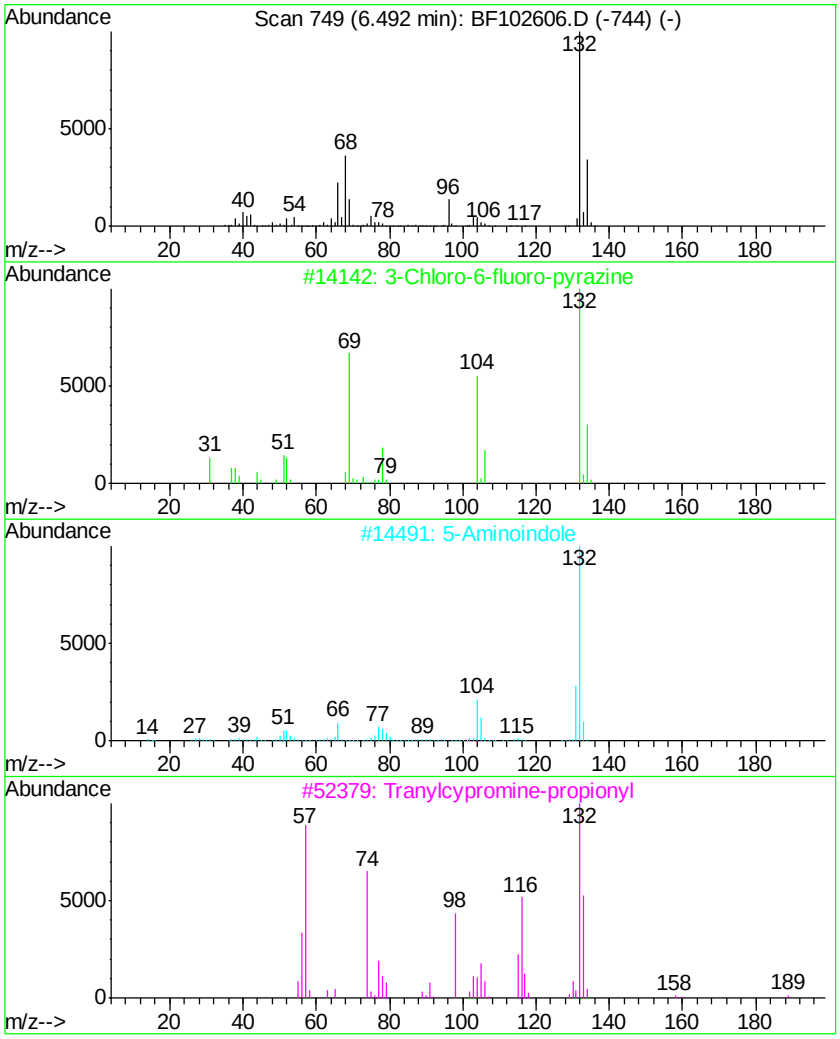
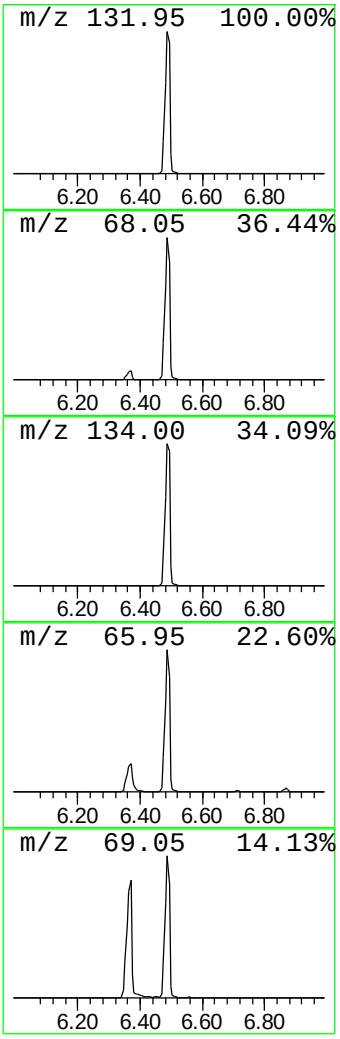
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	82.57 ng	4395820	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF102606.D
Acq On : 29 Jan 2018 19:28
Operator : SJ/JU
Sample : J1344-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-3-WW(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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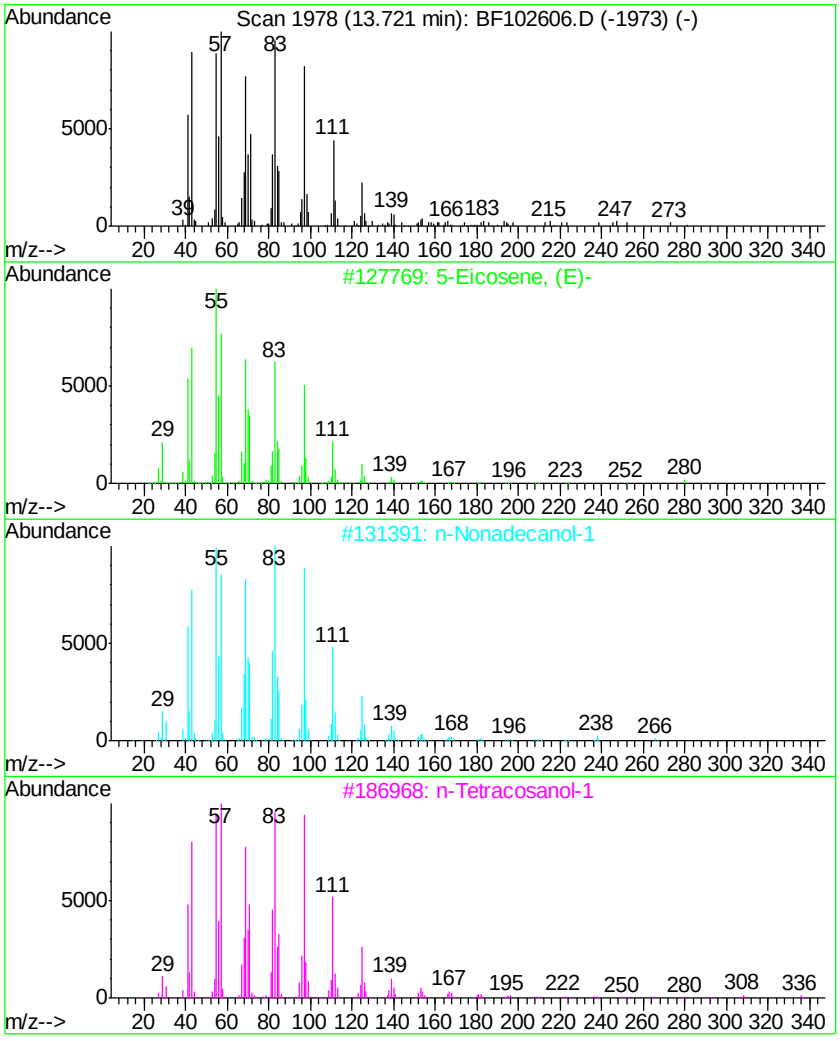
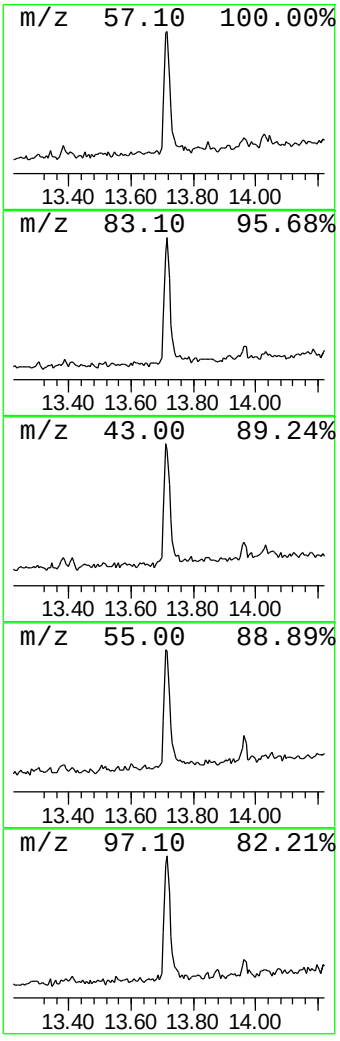
Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	7.18 ng	445656	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-SAN-3-WW(5-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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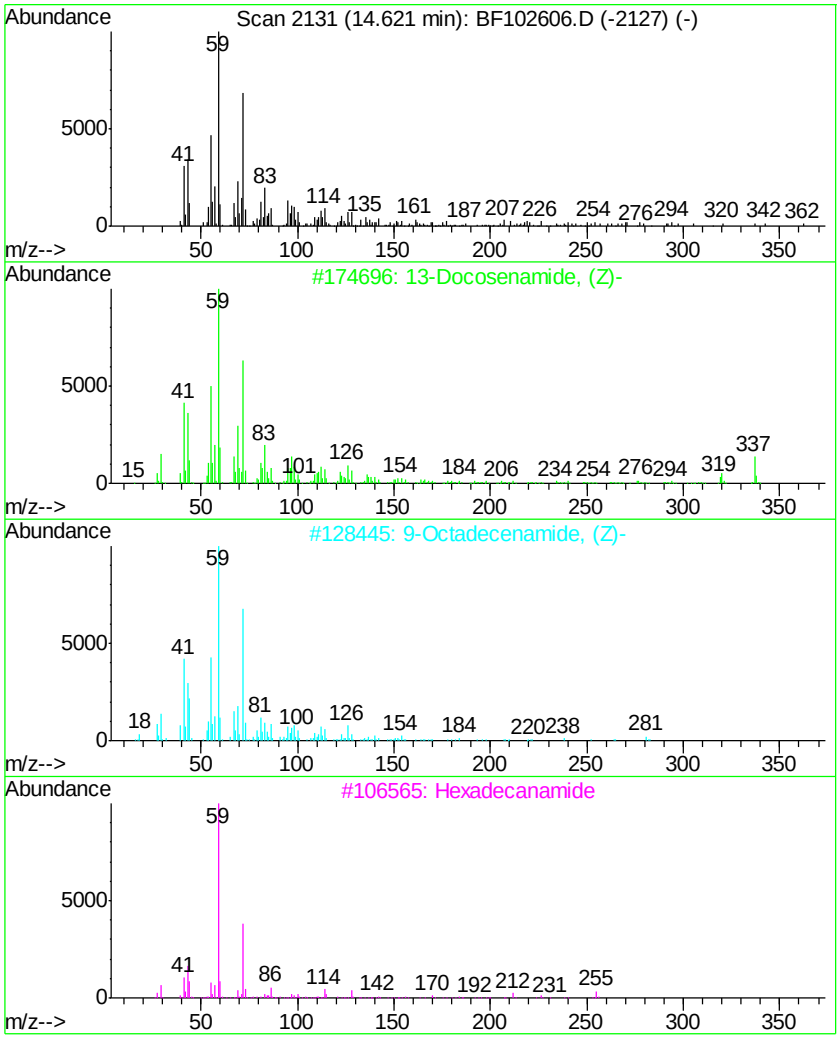
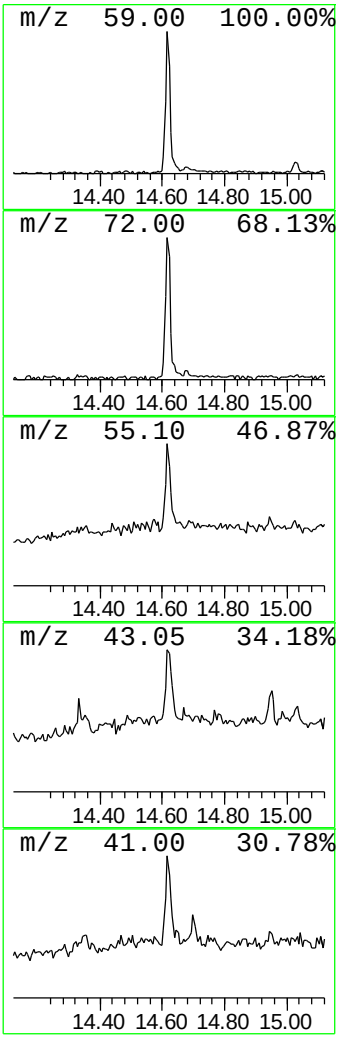
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	4.92 ng	250411	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	68
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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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...	4.93	2.5	ng	134516	1	6.71	1064750	20.0
unknown6.49	6.49	82.6	ng	4395820	1	6.71	1064750	20.0
5-Eicosene, (E)-	13.72	7.2	ng	445656	5	13.88	1240550	20.0
13-Docosenamide, ...	14.62	4.9	ng	250411	6	15.31	1018260	20.0