LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096915.D
Acq On : 20 Jul 2017 19:41
Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

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-BF071317.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	2.793	136	137	155	rBV	29014	86669	3.63%	0.438%
2	4.734	463	467	477	rBV	170653	240984	10.09%	1.218%
3	5.175	538	542	555	rBV	2021568	2109451	88.28%	10.666%
4	6.228	715	721	736	rBV	1930810	2081639	87.12%	10.525%
5	6.339	736	740	743	rBV	2140061	2027895	84.87%	10.253%
6	6.569	775	779	790	rBV	641900	579112	24.24%	2.928%
7	6.728	801	806	809	rBV	1541285	1518577	63.55%	7.678%
8	6.751	809	810	822	rVB	41047	42020	1.76%	0.212%
9	7.133	870	875	878	rBV	1368934	1266209	52.99%	6.402%
10	7.263	892	897	905	rVB	33021	40097	1.68%	0.203%
11	7.769	980	983	990	rBV	29621	29820	1.25%	0.151%
12	7.851	993	997	1000	rBV	894053	732787	30.67%	3.705%
13	8.933	1175	1181	1184	rBV	2401485	2389503	100.00%	12.082%
14	9.327	1244	1248	1251	rBV	443556	369647	15.47%	1.869%
15	9.598	1290	1294	1298	rBV2	990791	822232	34.41%	4.157%
16	10.386	1423	1428	1431	rBV	1307852	1220038	51.06%	6.169%
17	10.521	1448	1451	1458	rVB	44633	46986	1.97%	0.238%
18	10.969	1523	1527	1529	rBV2	34035	28920	1.21%	0.146%
19	11.074	1541	1545	1548	rBV	854247	701973	29.38%	3.549%
20	11.321	1584	1587	1593	rVB	181110	167240	7.00%	0.846%
21	12.133	1722	1725	1731	rBV	283712	290632	12.16%	1.469%
22	12.280	1747	1750	1754	rBV	28216	26981	1.13%	0.136%
23	12.504	1784	1788	1790	rBV2	41392	40456	1.69%	0.205%
24	12.657	1810	1814	1818	rBV	1585748	1623849	67.96%	8.211%
25	13.115	1889	1892	1898	rBV4	26667	41099	1.72%	0.208%
26	13.221	1905	1910	1913	rBV6	22417	47206	1.98%	0.239%
27	13.568	1966	1969	1977	rVB	86593	113367	4.74%	0.573%
28	13.698	1987	1991	1995	rBV	570901	561480	23.50%	2.839%
29	14.492	2124	2126	2134	rBV7	34162	67235	2.81%	0.340%
30	15.068	2220	2224	2229	rBV	416671	463577	19.40%	2.344%

Sum of corrected areas: 19777681

LSC Report - Integrated Chromatogram

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Data File : BF096915.D
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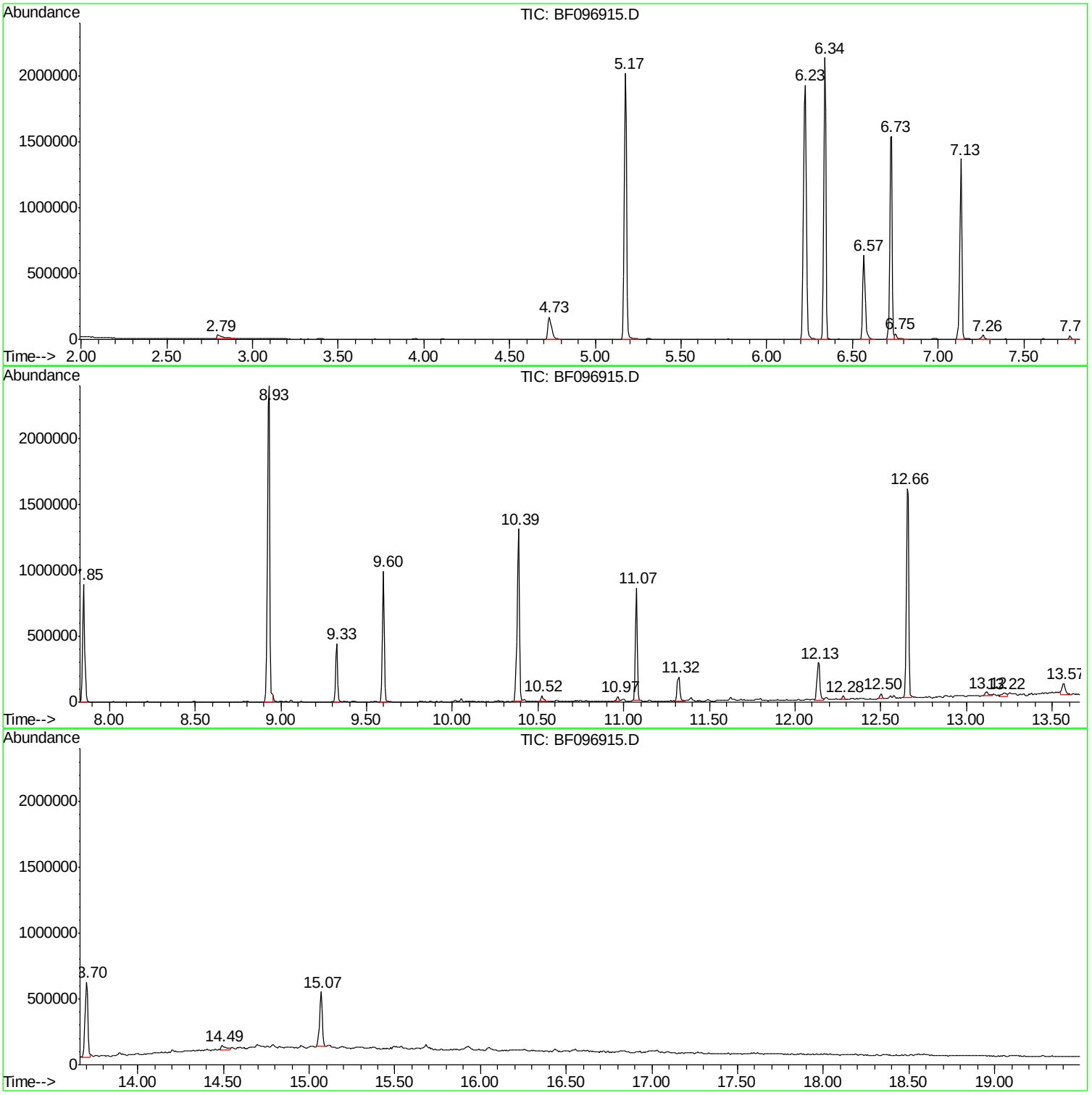
Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096915.D
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Operator : SJ/JU
Sample : I4312-01
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Instrument : BNA_F
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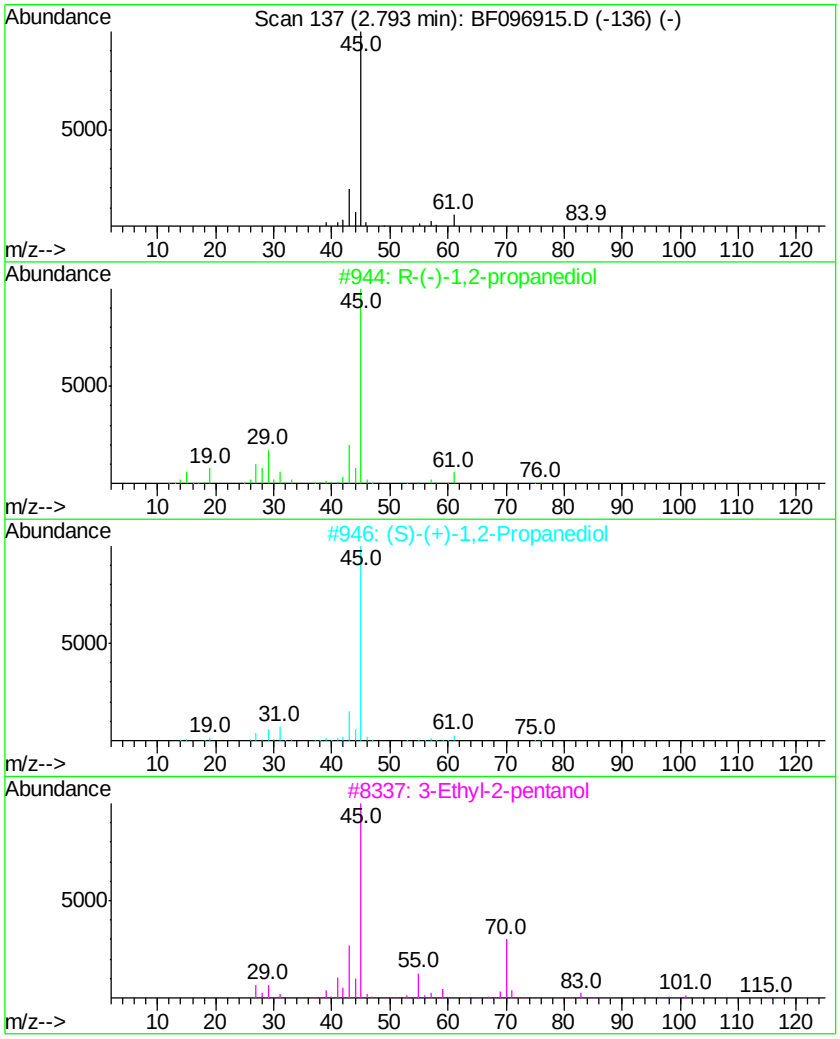
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

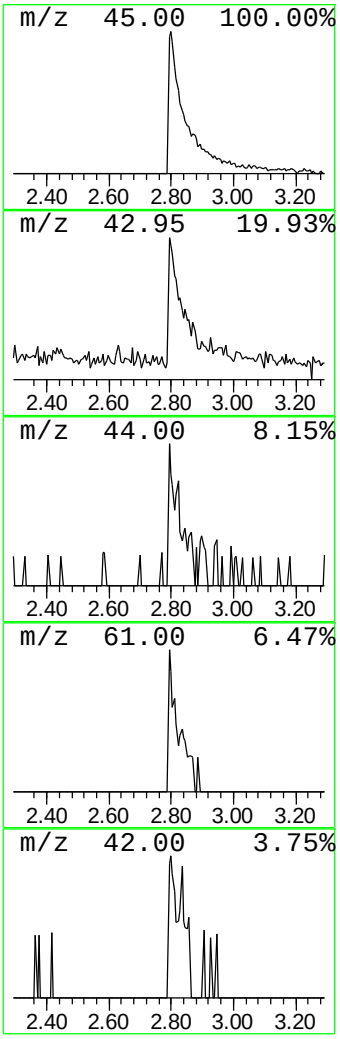
****

Peak Number 1 unknown2.79 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	2.99 ng	86669	1,4-Dichlorobenzene-d4	6.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Heptanol	116	C7H16O	000543-49-7	9





Library Search Compound Report

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Data File : BF096915.D
Acq On : 20 Jul 2017 19:41
Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

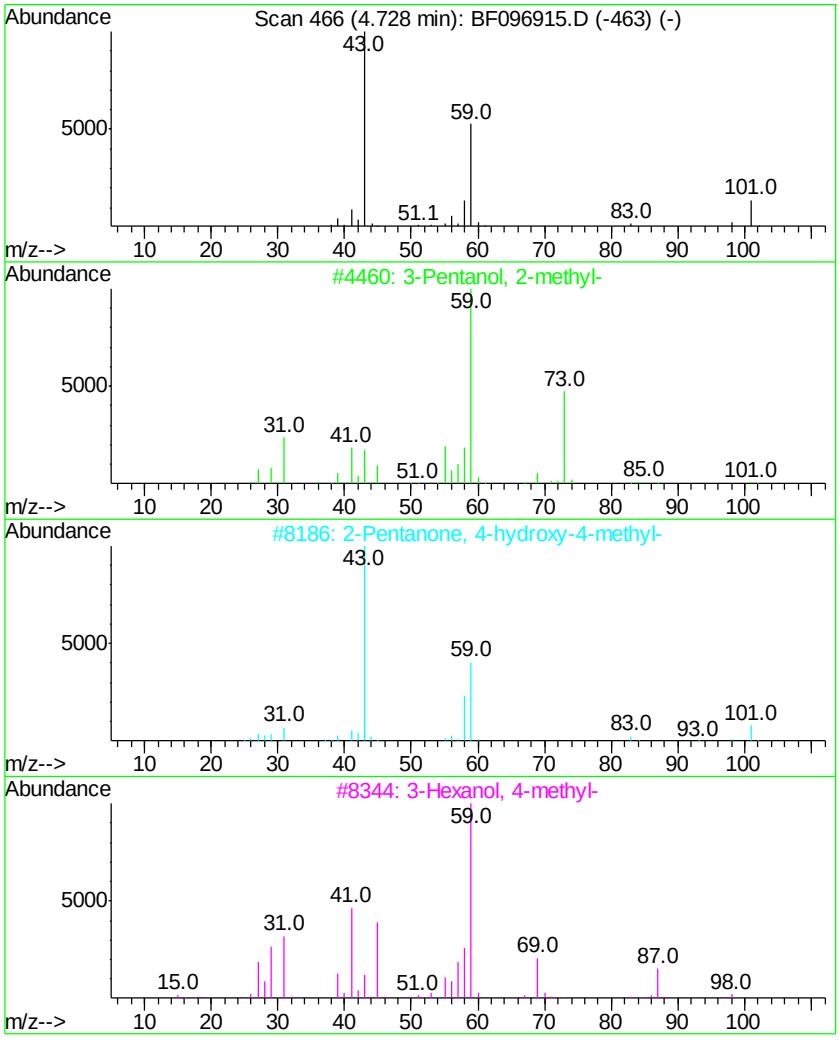
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

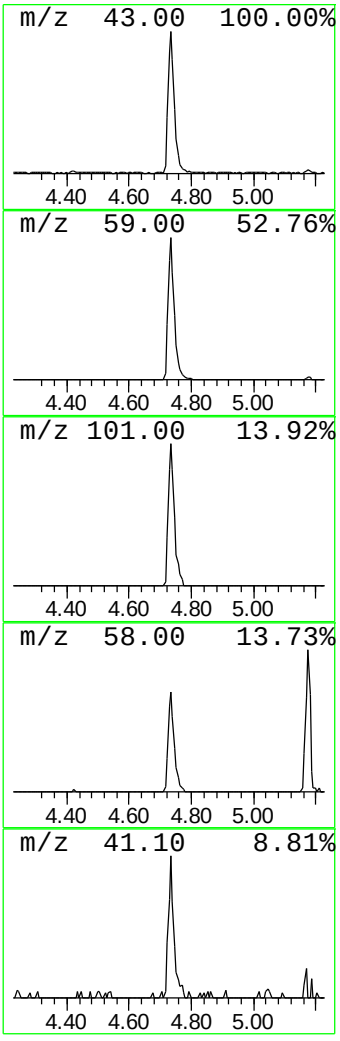
****

Peak Number 2 3-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	8.32 ng	240984	1,4-Dichlorobenzene-d4	6.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
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Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

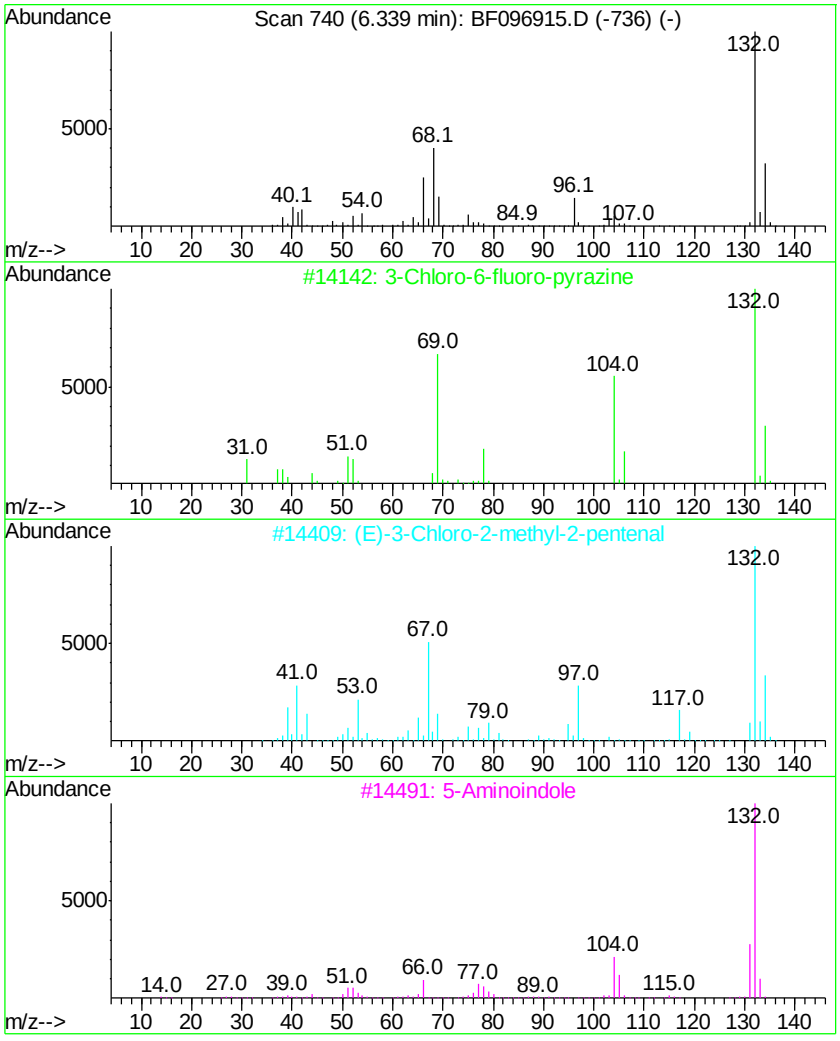
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

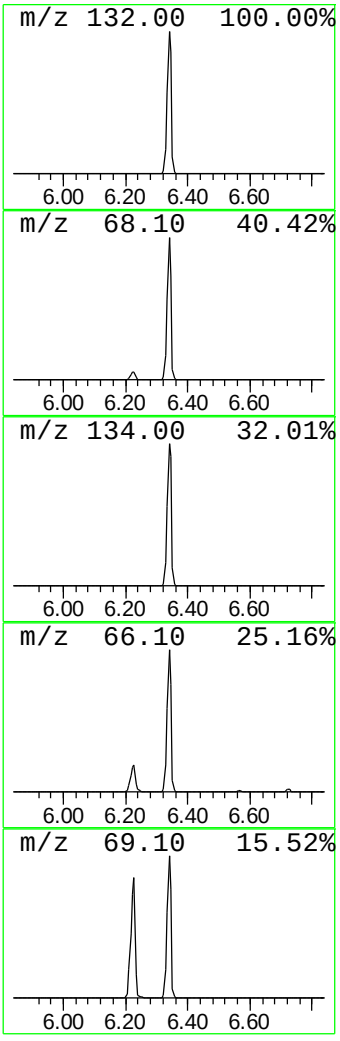
****

Peak Number 3 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	70.03 ng	2027900	1,4-Dichlorobenzene-d4	6.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096915.D
Acq On : 20 Jul 2017 19:41
Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

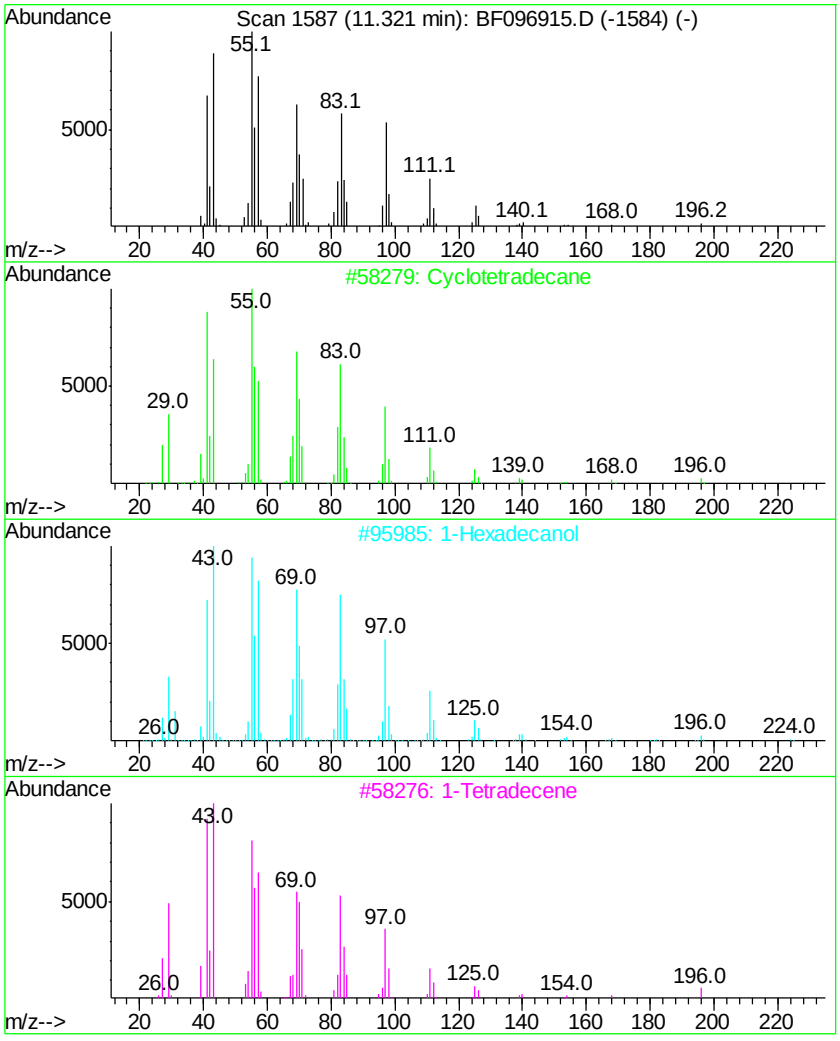
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

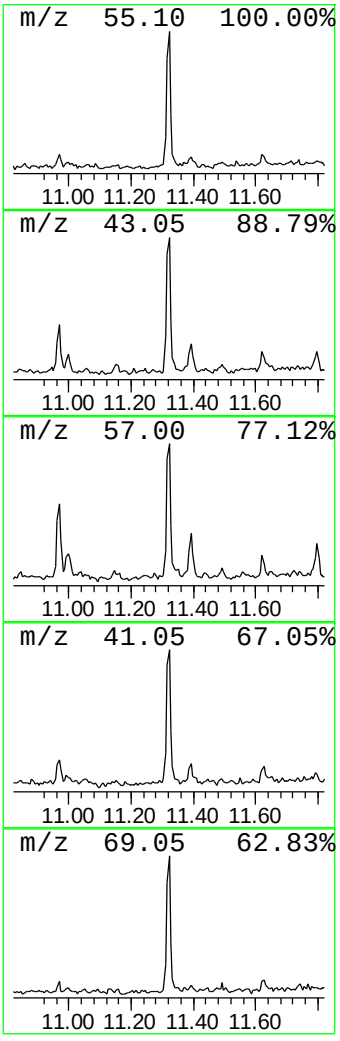
****

Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.32	4.76 ng	167240	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	95
3	1-Tetradecene	196	C14H28	001120-36-1	95
4	n-Pentadecanol	228	C15H32O	000629-76-5	94
5	Cetene	224	C16H32	000629-73-2	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
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Acq On : 20 Jul 2017 19:41
Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

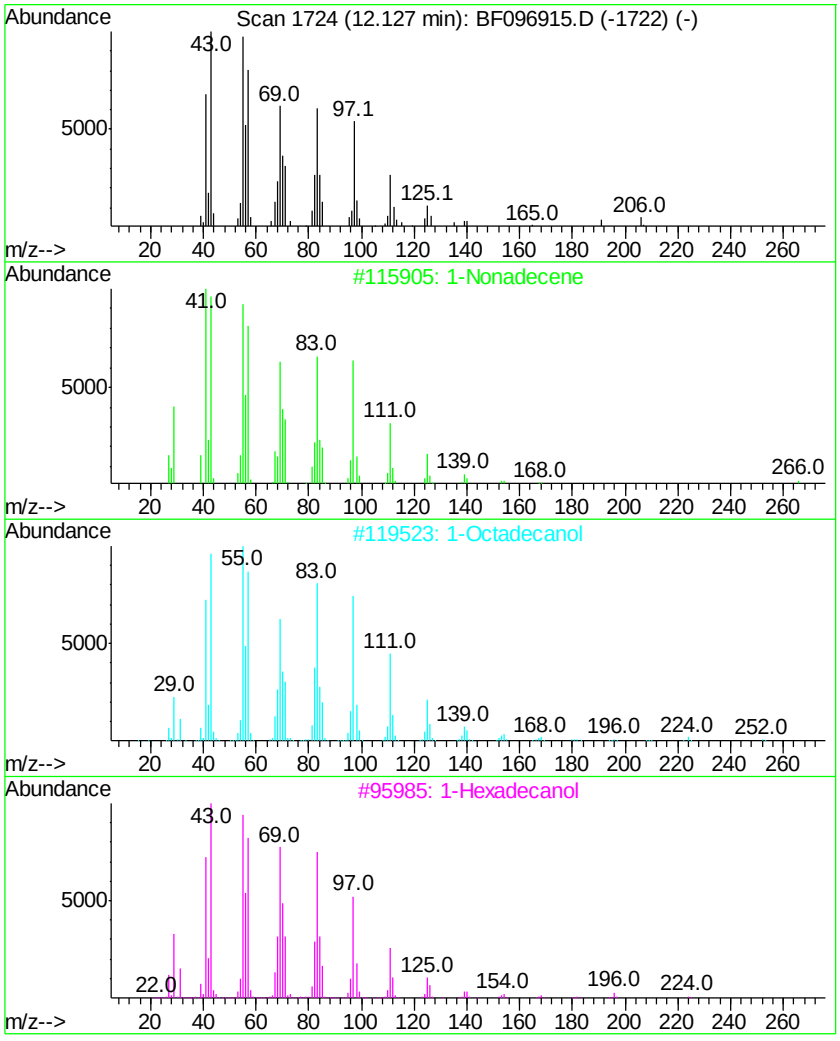
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

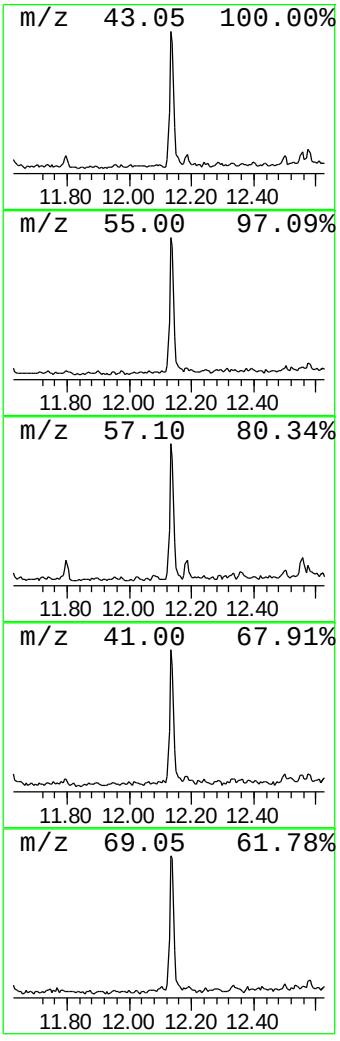
****

Peak Number 6 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	8.28 ng	290632	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	Cetene	224	C16H32	000629-73-2	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90





Library Search Compound Report

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Operator : SJ/JU
Sample : I4312-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-209

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

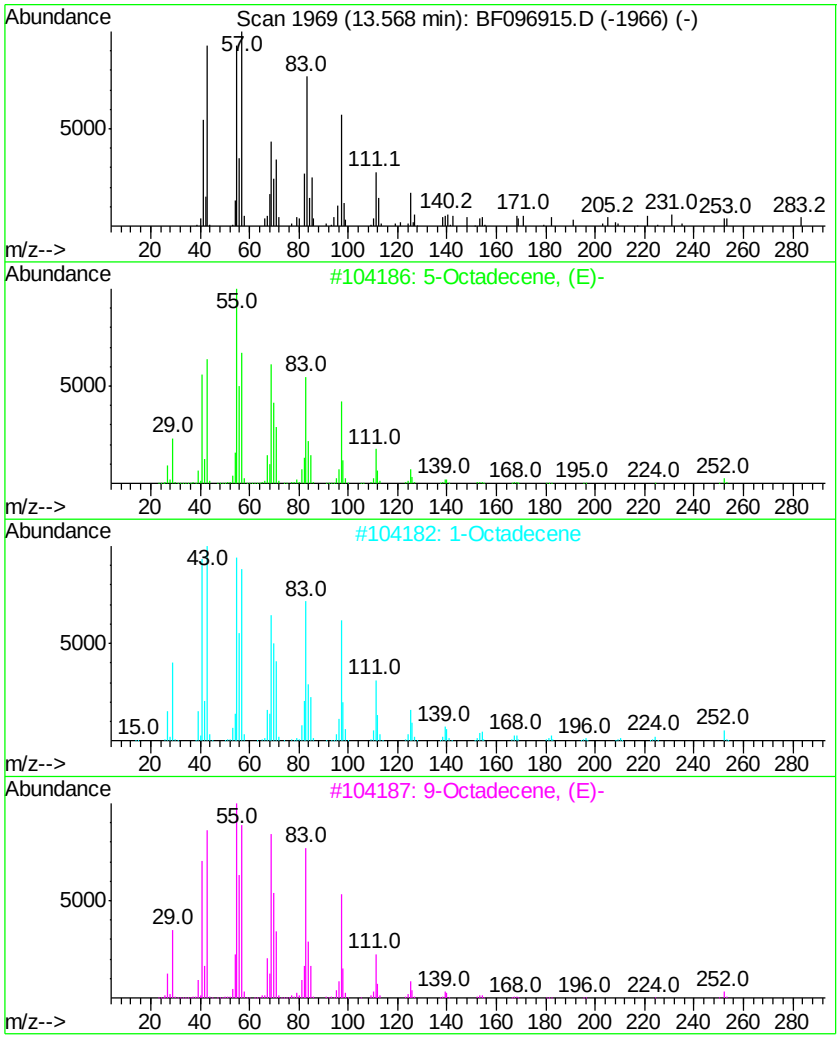
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

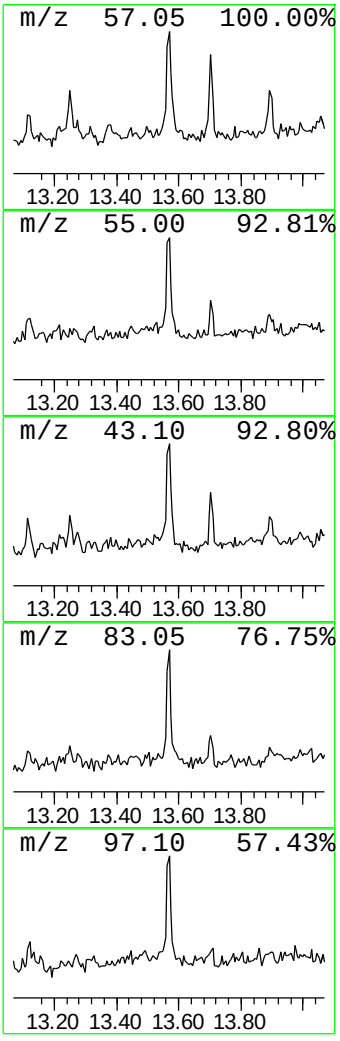
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	4.04 ng	113367	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	1-Octadecene	252	C18H36	000112-88-9	93
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	87
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	87
5	Behenic alcohol	326	C22H46O	000661-19-8	76





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Sample : I4312-01
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

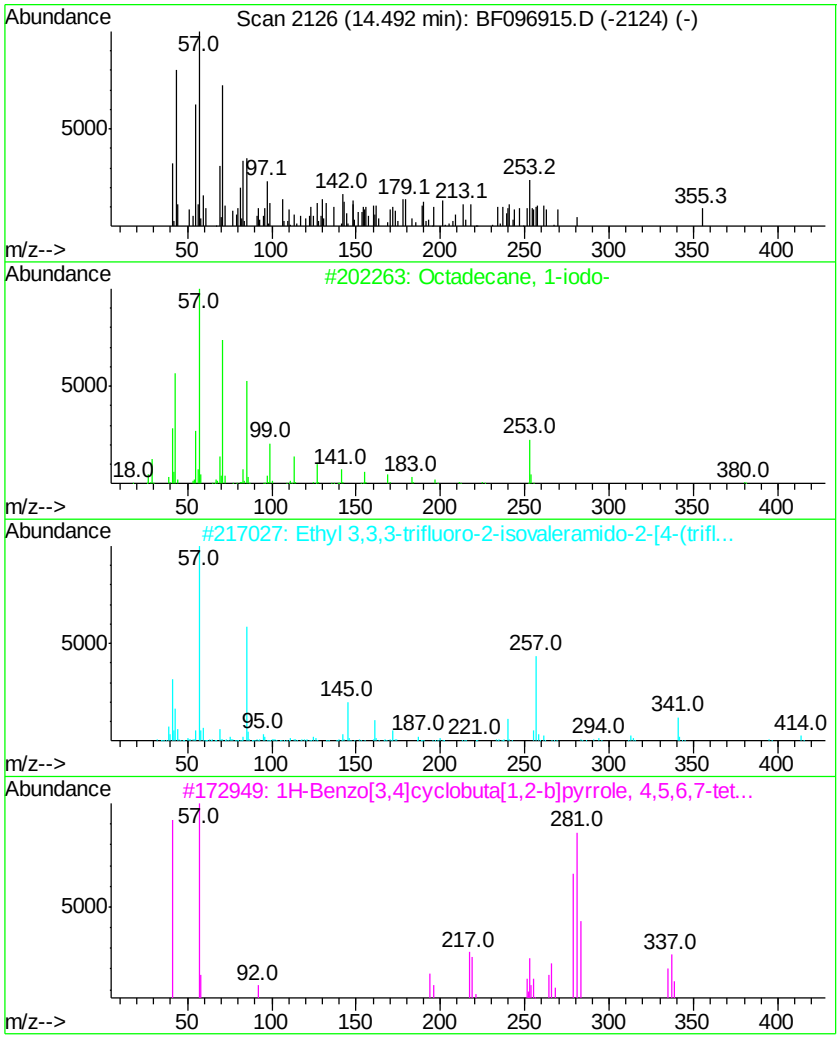
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

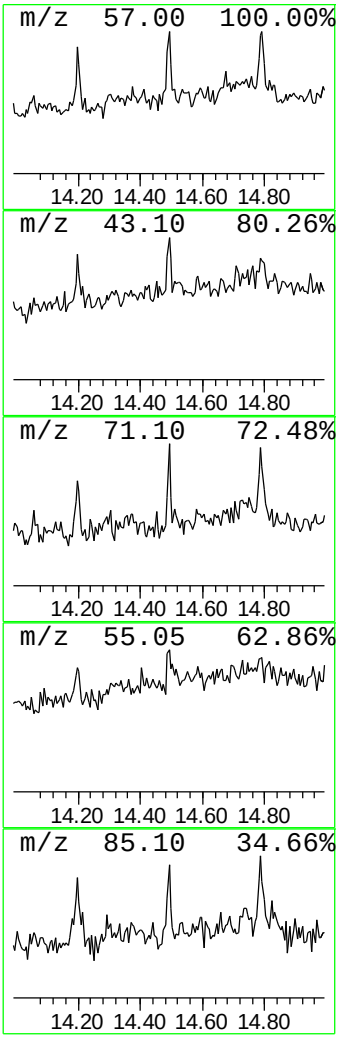
****

Peak Number 8 unknown14.49 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.90 ng	67235	Perylene-d12	15.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	10
2	Ethyl 3,3,3-trifluoro-2-isovaler...	414	C17H20F6N2O3	1000224-19-8	9
3	1H-Benzo[3,4]cyclobuta[1,2-b]pyr...	335	C14H13Cl4N	060857-30-9	7
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	7
5	Methyl 11-acetoxyhexadecanoate	328	C19H36O4	088167-64-0	7





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.79	2.79	3.0	ng	86669	1	6.57	579112	20.0
3-Pentanol, 2-met...	4.73	8.3	ng	240984	1	6.57	579112	20.0
unknown6.34	6.34	70.0	ng	2027900	1	6.57	579112	20.0
Cyclotetradecane	11.32	4.8	ng	167240	4	11.07	701973	20.0
1-Nonadecene	12.13	8.3	ng	290632	4	11.07	701973	20.0
5-Octadecene, (E)-	13.57	4.0	ng	113367	5	13.70	561480	20.0
unknown14.49	14.49	2.9	ng	67235	6	15.07	463577	20.0