LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

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-BF122116.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	1.924	9	12	16	rVB3	31669	82402	1.47%	0.187%
2	3.798	174	176	177	rBV	46349	74068	1.32%	0.168%
3	3.821	177	178	186	rVB	127348	225927	4.04%	0.513%
4	4.701	252	255	265	rVB	1337872	1997238	35.71%	4.535%
5	5.170	293	296	306	rBV	3878339	4086535	73.06%	9.280%
6	5.410	314	317	320	rBV	108141	165193	2.95%	0.375%
7	5.513	325	326	334	rVB2	57978	95748	1.71%	0.217%
8	6.244	387	390	396	rBV2	4064468	5593454	100.00%	12.702%
9	6.347	396	399	401	rVV	4758586	4547764	81.31%	10.327%
10	6.416	404	405	408	rVB	59301	56406	1.01%	0.128%
11	6.576	417	419	421	rBV	1001885	1133937	20.27%	2.575%
12	6.724	430	432	435	rBV	2657426	3023521	54.05%	6.866%
13	6.862	443	444	448	rBV2	195717	212188	3.79%	0.482%
14	7.022	452	458	466	rBV3	163498	481095	8.60%	1.093%
15	7.147	466	469	471	rBV	2467673	2699953	48.27%	6.131%
16	7.650	511	513	519	rBV4	54503	109776	1.96%	0.249%
17	7.856	529	531	534	rVB	1153547	1243977	22.24%	2.825%
18	8.256	564	566	570	rBV2	31116	56134	1.00%	0.127%
19	8.942	623	626	628	rBV	4441108	4433779	79.27%	10.069%
20	9.342	659	661	663	rBV	572188	496443	8.88%	1.127%
21	9.605	682	684	688	rVB	1371605	1486335	26.57%	3.375%
22	10.062	722	724	726	rVB	55020	60809	1.09%	0.138%
23	10.393	751	753	756	rBV2	2009449	2618650	46.82%	5.947%
24	10.531	763	765	769	rVB	108050	137503	2.46%	0.312%
25	10.976	802	804	805	rBV	103838	94612	1.69%	0.215%
26	11.079	811	813	816	rBV	1051883	1374225	24.57%	3.121%
27	11.399	839	841	844	rVB	134354	121234	2.17%	0.275%
28	11.639	860	862	866	rBV2	78430	103832	1.86%	0.236%
29	12.668	949	952	955	rBV	3501361	4167198	74.50%	9.463%
30	13.159	989	995	1000	rBV	90624	178305	3.19%	0.405%
31	13.594	1030	1033	1041	rBV	74573	185083	3.31%	0.420%
32	13.708	1041	1043	1046	rBV	1328878	1236211	22.10%	2.807%
33	14.474	1107	1110	1114	rBV	367197	384608	6.88%	0.873%
34	14.554	1115	1117	1120	rVB	64497	84133	1.50%	0.191%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.068	1159	1162	1164	rBV	684873	987841	17.66%	2.243%

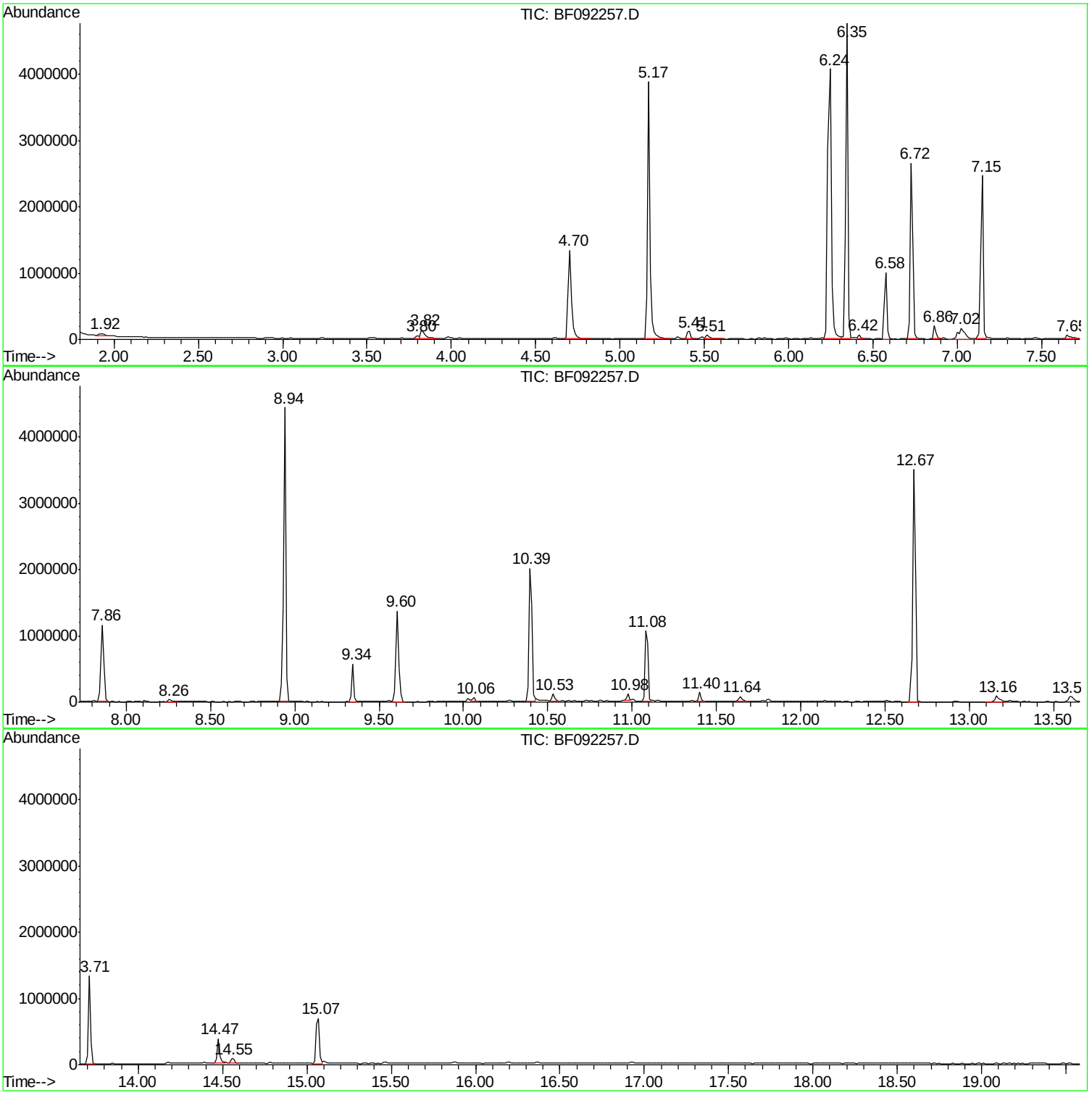
Sum of corrected areas: 44036117

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

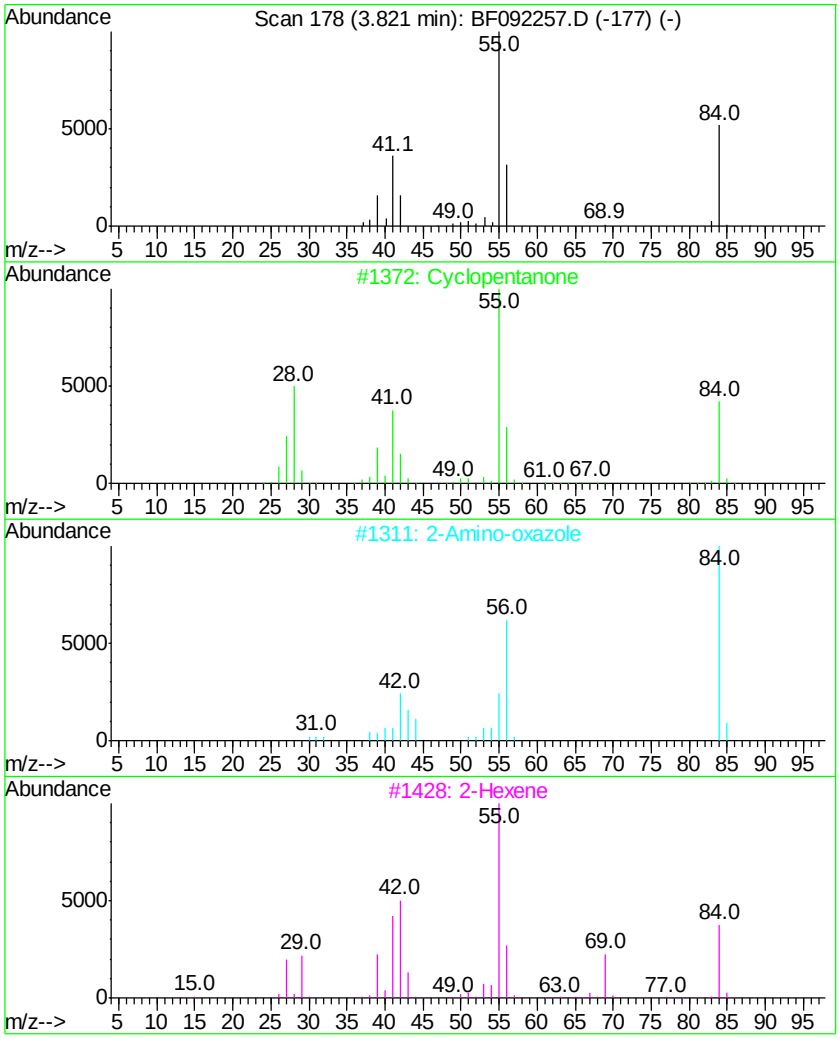
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

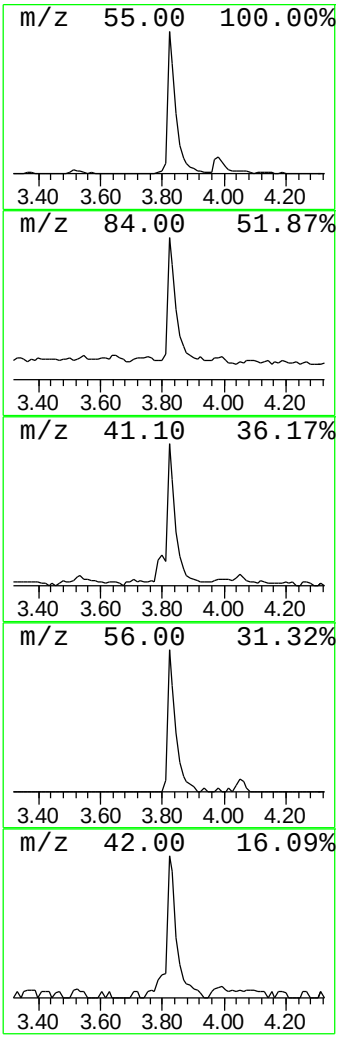
****

Peak Number 1 Cyclopentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.82	3.98 ng	225927	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	86
2	2-Amino-oxazole	84	C3H4N2O	004570-45-0	59
3	2-Hexene	84	C6H12	000592-43-8	42
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	9
5	2(5H)-Furanone	84	C4H4O2	000497-23-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

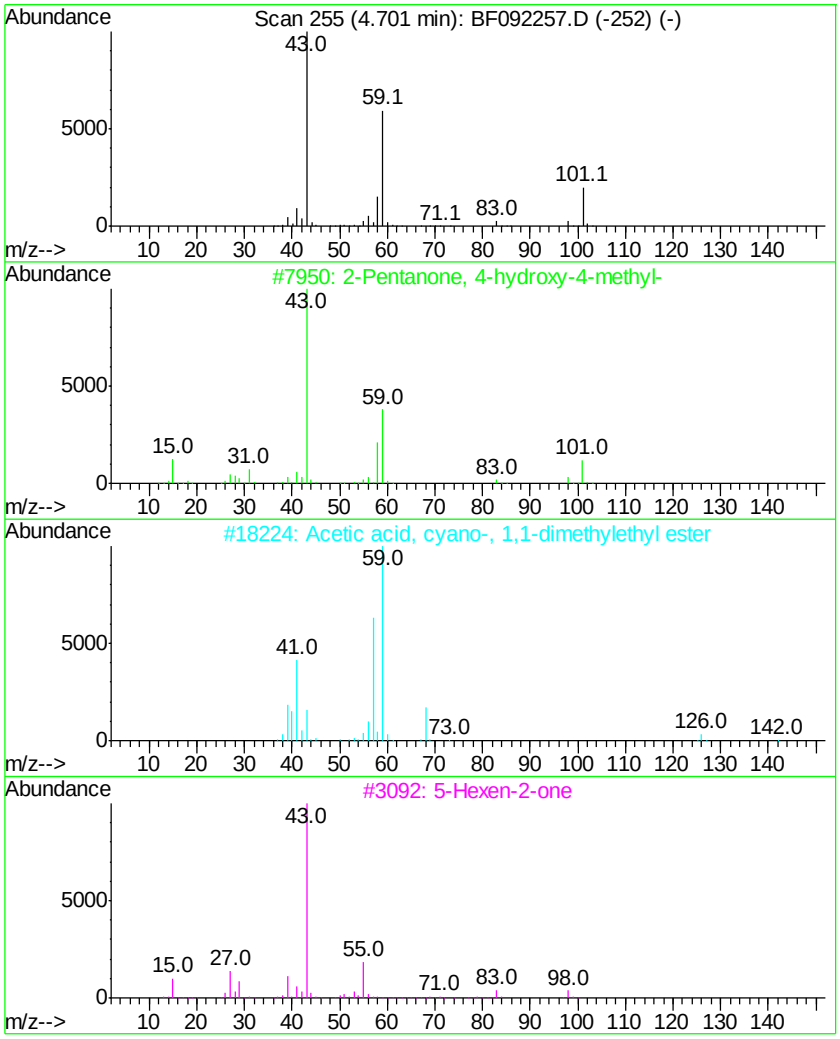
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

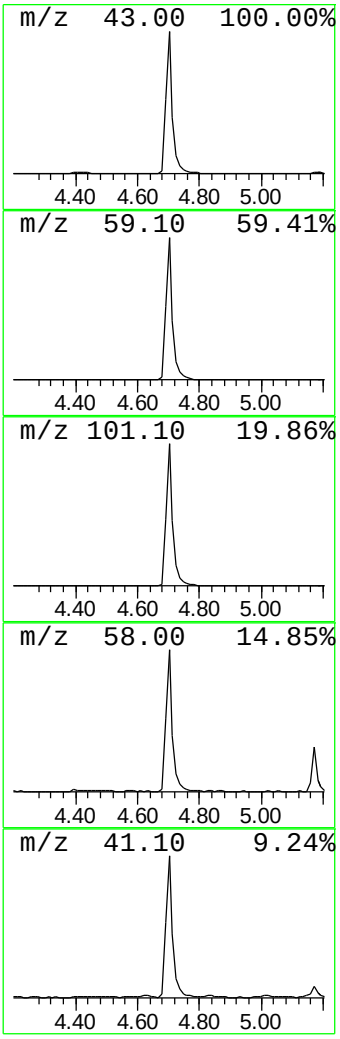
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	35.23 ng	1997240	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

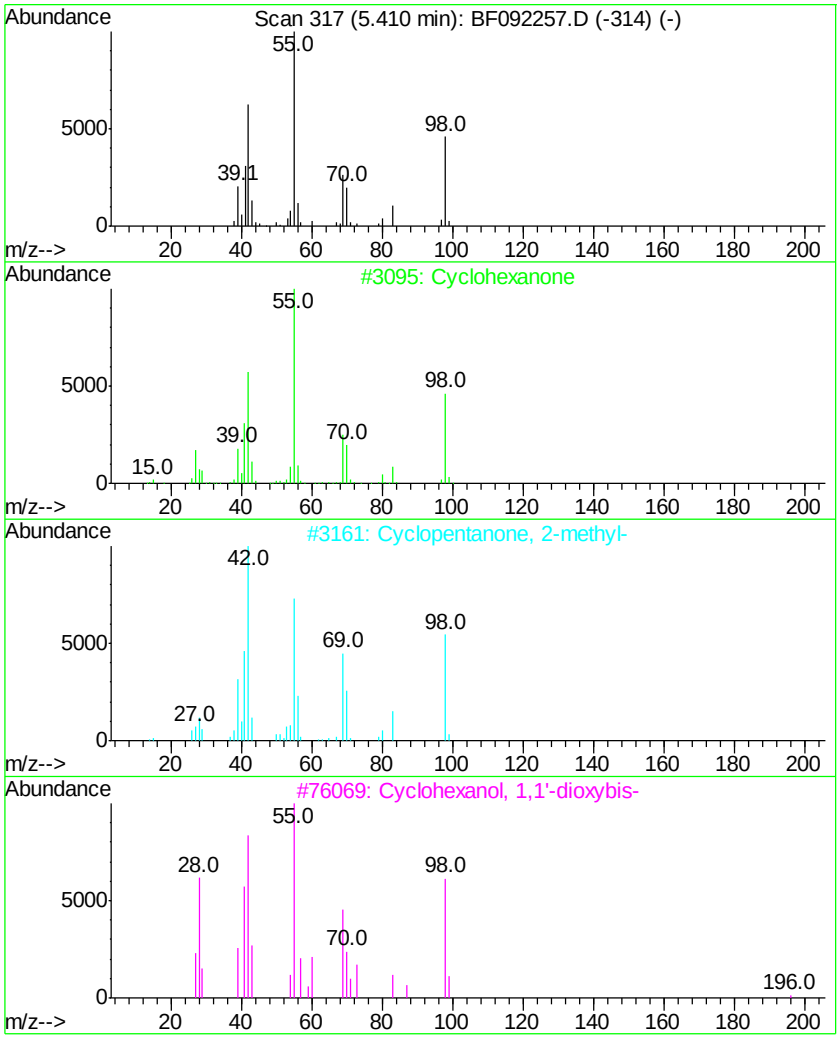
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

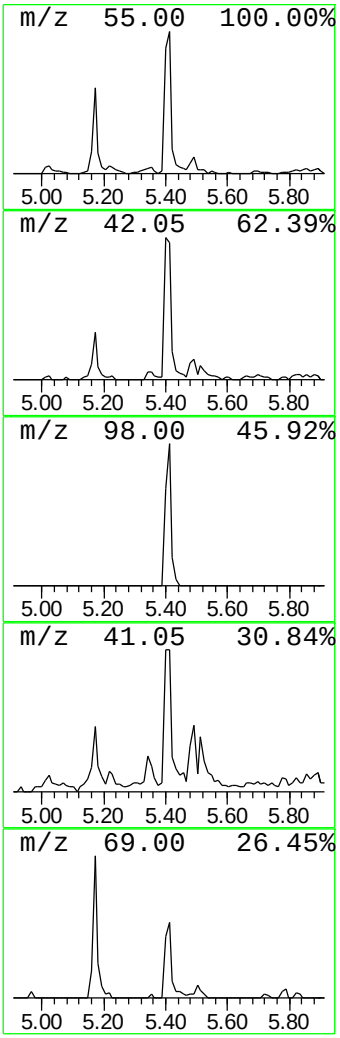
****

Peak Number 3 Cyclohexanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.41	2.91 ng	165193	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	94
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	59
3	Cyclohexanol, 1,1'-dioxybis-	230	C12H22O4	002407-94-5	56
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	40
5	1-Pentene	70	C5H10	000109-67-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

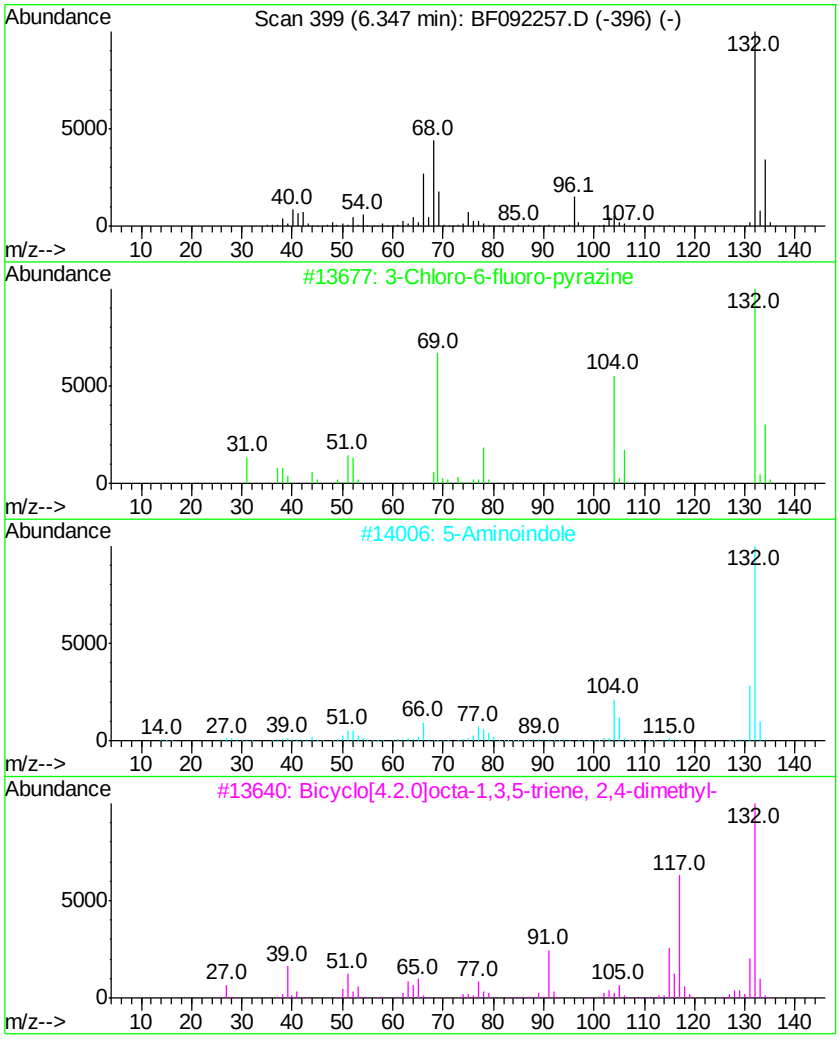
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

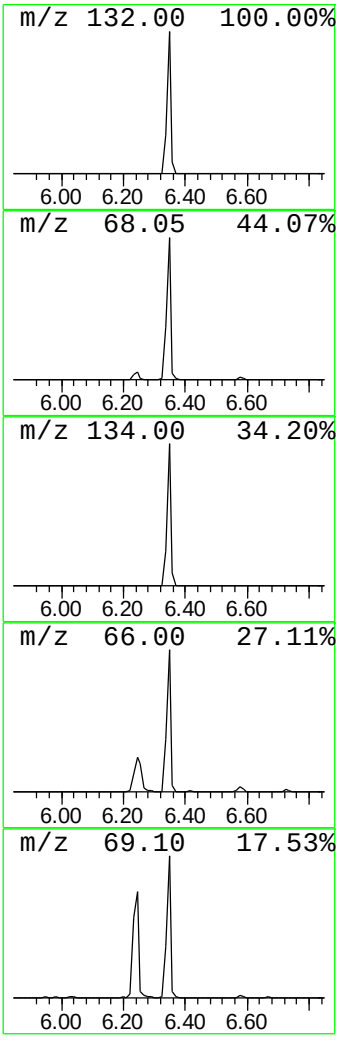
****

Peak Number 4 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	80.21 ng	4547760	1,4-Dichlorobenzene-d4	6.58

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

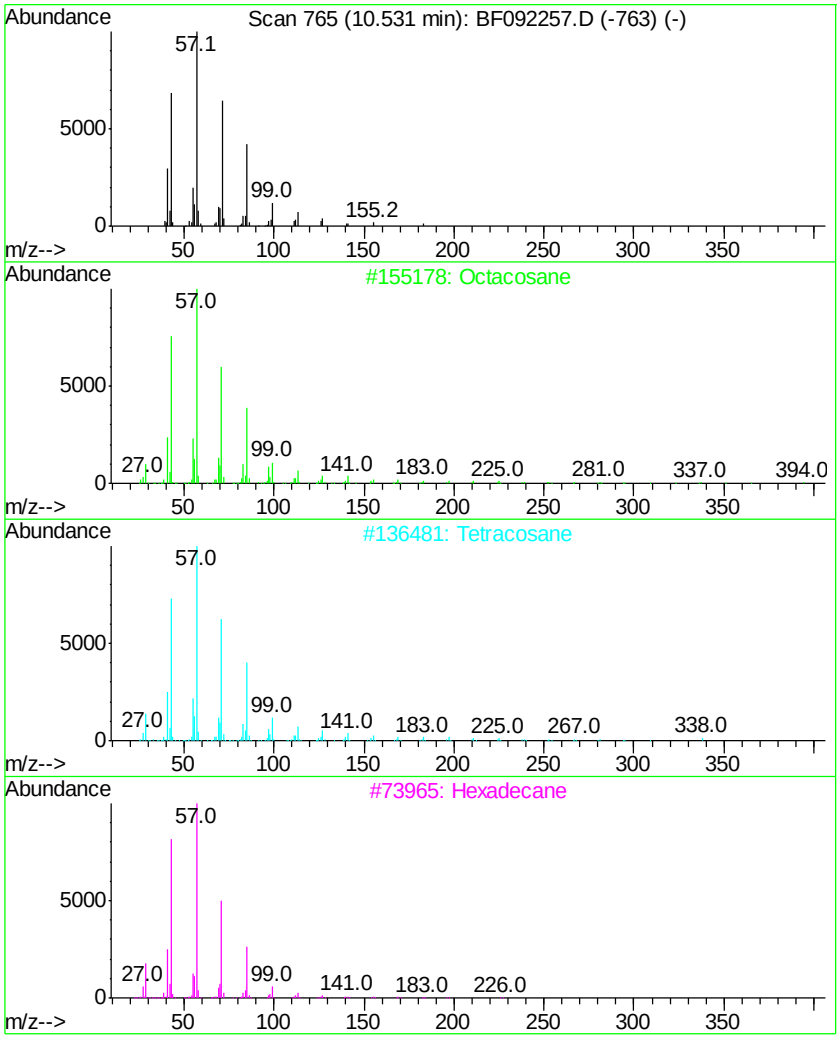
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

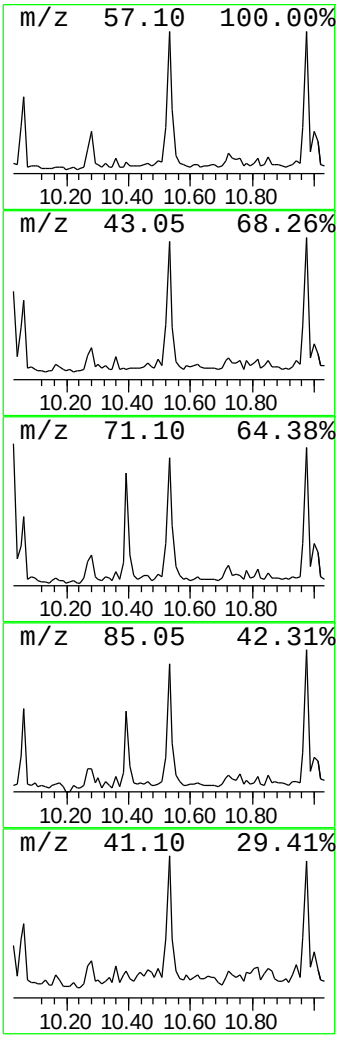
****

Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	2.00 ng	137503	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5	Octadecane	254	C18H38	000593-45-3	86





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Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

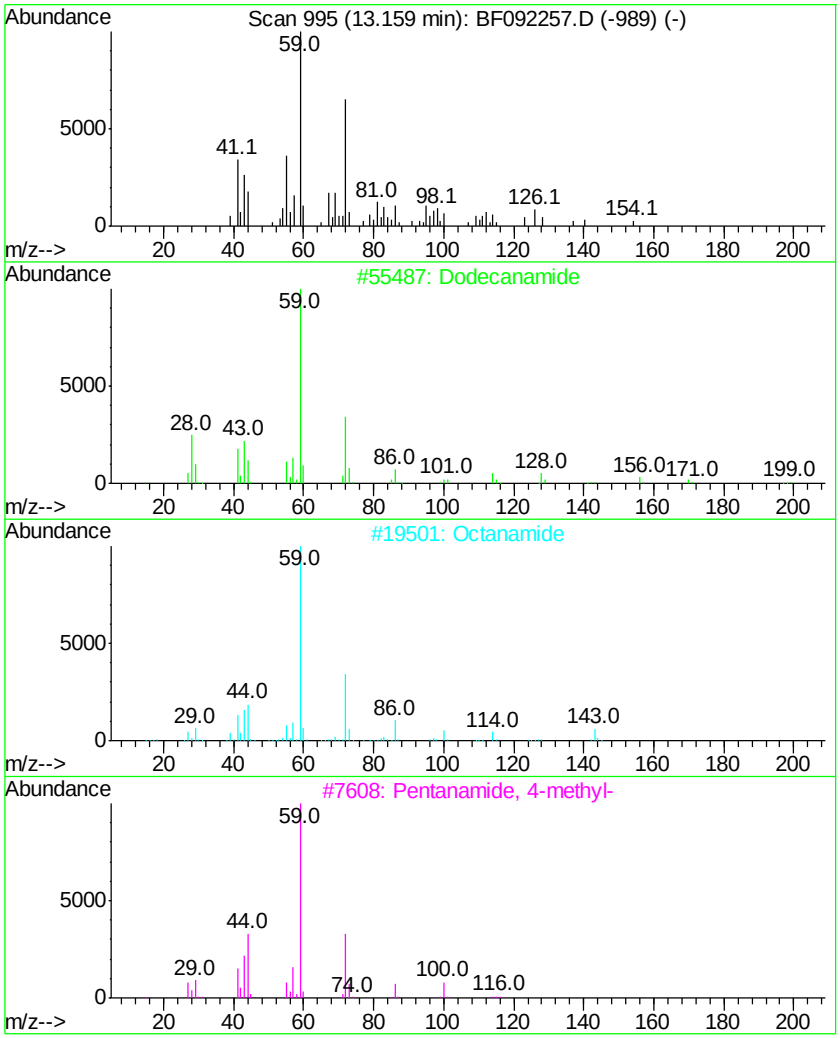
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

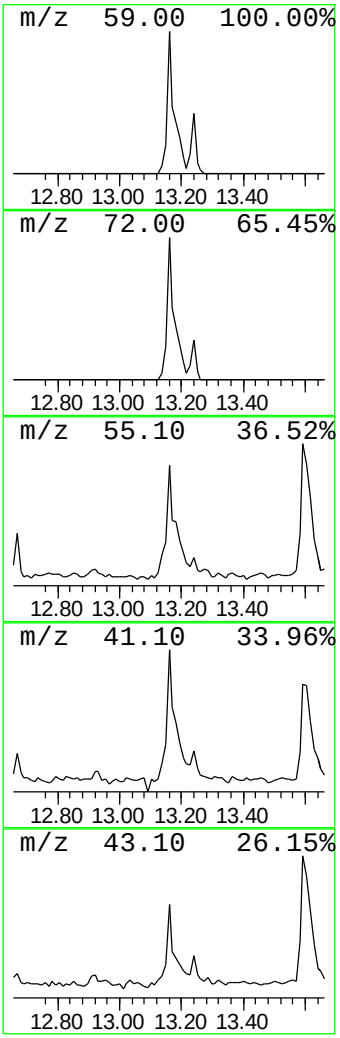
****

Peak Number 7 Dodecanamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	2.88 ng	178305	Chrysene-d12	13.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide	199	C12H25NO	001120-16-7	59
2	Octanamide	143	C8H17NO	000629-01-6	53
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	45
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	45
5	2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

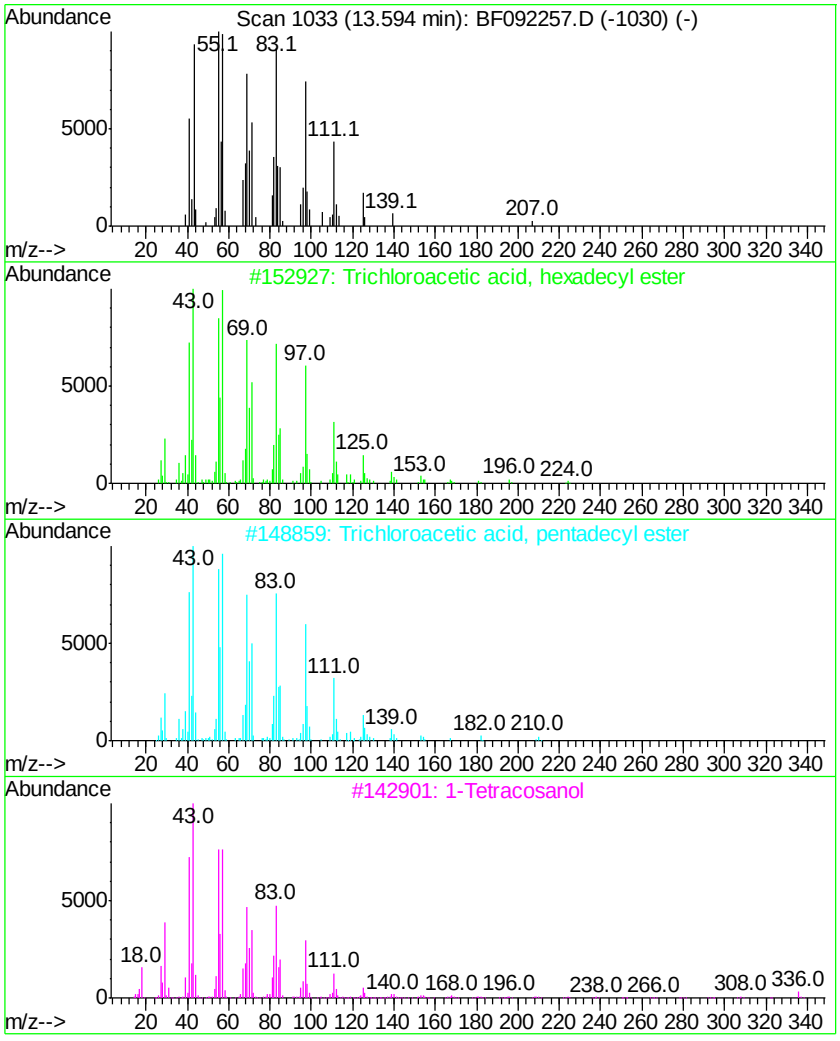
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

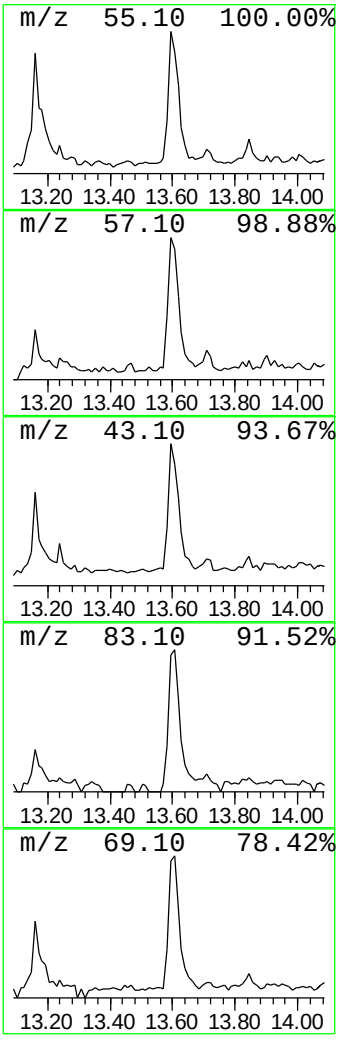
****

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	2.99 ng	185083	Chrysene-d12	13.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	1-Tetracosanol	354	C24H50O	000506-51-4	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	1-Nonadecene	266	C19H38	018435-45-5	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092257.D
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Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

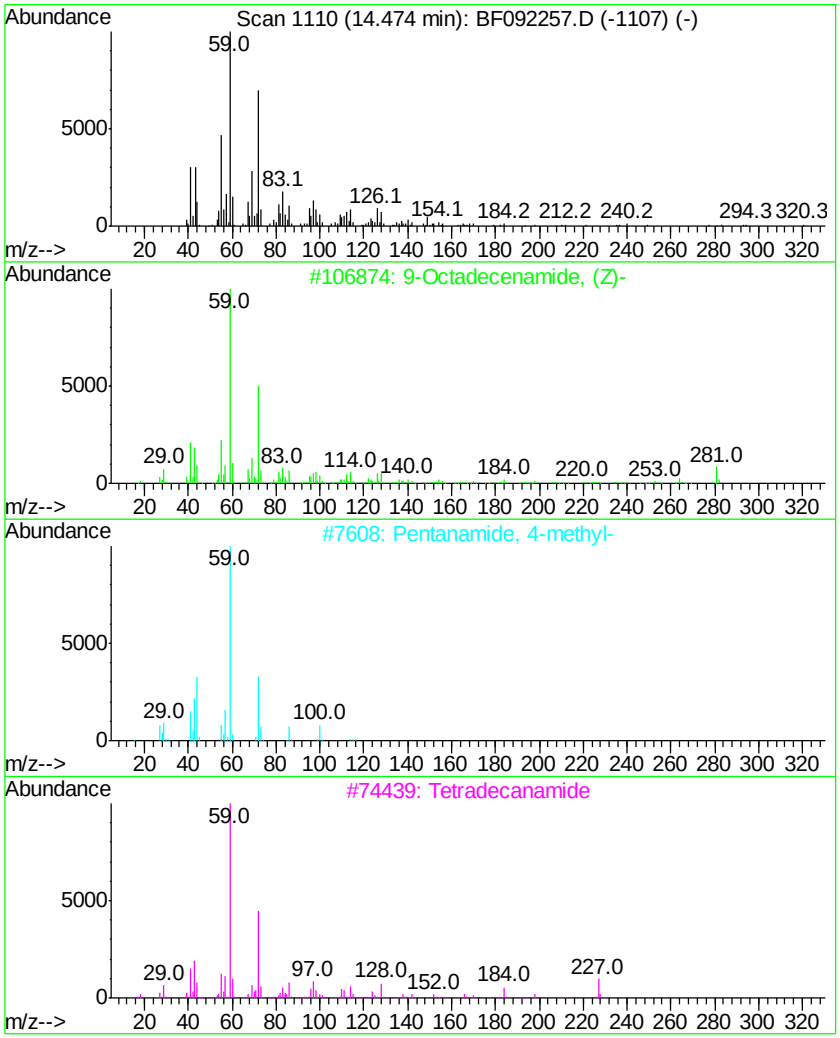
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

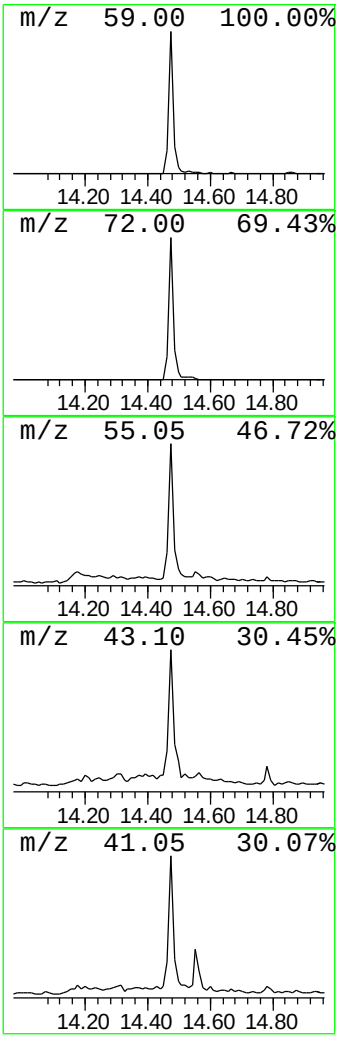
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	7.79 ng	384608	Perylene-d12	15.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	56
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092257.D
Acq On : 13 Jan 2017 22:24
Operator : UM/SJ
Sample : I1182-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-SB-78-80

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentanone	3.82	4.0	ng	225927	1	6.58	1133940	20.0
2-Pentanone, 4-hy...	4.70	35.2	ng	1997240	1	6.58	1133940	20.0
Cyclohexanone	5.41	2.9	ng	165193	1	6.58	1133940	20.0
unknown6.35	6.35	80.2	ng	4547760	1	6.58	1133940	20.0
Octacosane	10.53	2.0	ng	137503	4	11.08	1374230	20.0
Dodecanamide	13.16	2.9	ng	178305	5	13.71	1236210	20.0
Trichloroacetic a...	13.59	3.0	ng	185083	5	13.71	1236210	20.0
9-Octadecenamide,...	14.47	7.8	ng	384608	6	15.07	987841	20.0