LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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	3.947	184	189	196	rVB	101456	197412	3.20%	0.466%
2	4.084	196	201	205	rBV2	51294	107471	1.74%	0.254%
3	4.656	249	251	259	rVB	377021	561859	9.10%	1.325%
4	5.136	291	293	302	rBV	1854796	2434696	39.44%	5.744%
5	5.513	322	326	330	rBV2	63622	128763	2.09%	0.304%
6	5.673	338	340	343	rBV3	73606	147508	2.39%	0.348%
7	5.959	362	365	367	rVB2	57431	90867	1.47%	0.214%
8	6.222	385	388	395	rBV	893933	1493791	24.20%	3.524%
9	6.324	395	397	400	rBV	4532674	4278919	69.31%	10.094%
10	6.553	415	417	420	rBV	1095500	1012835	16.41%	2.389%
11	6.713	428	431	433	rBV	3138101	4038339	65.41%	9.527%
12	7.125	464	467	470	rBV	2769737	3025067	49.00%	7.136%
13	7.182	470	472	476	rVB3	37478	71527	1.16%	0.169%
14	7.845	528	530	532	rBV	1477369	1638122	26.53%	3.864%
15	8.919	621	624	627	rBV	5825651	6173686	100.00%	14.564%
16	9.090	637	639	643	rVB4	47223	64628	1.05%	0.152%
17	9.319	657	659	661	rBV	106724	111927	1.81%	0.264%
18	9.582	680	682	685	rVB	1613556	1717891	27.83%	4.053%
19	10.382	749	752	754	rBV	2823393	3781866	61.26%	8.922%
20	10.496	760	762	767	rVB2	277374	361451	5.85%	0.853%
21	10.954	799	802	803	rBV	88915	89178	1.44%	0.210%
22	11.068	809	812	814	rBV	1306204	1716822	27.81%	4.050%
23	11.285	829	831	837	rVB	97381	169729	2.75%	0.400%
24	11.376	837	839	841	rVB	80302	67593	1.09%	0.159%
25	11.616	858	860	865	rBV2	138890	195483	3.17%	0.461%
26	12.394	926	928	930	rBV	68428	108835	1.76%	0.257%
27	12.439	930	932	935	rVB	128054	167933	2.72%	0.396%
28	12.657	947	951	953	rBV	3900852	5813221	94.16%	13.714%
29	13.228	999	1001	1003	rBV2	97051	100783	1.63%	0.238%
30	13.445	1017	1020	1028	rBV	49836	77613	1.26%	0.183%
31	13.571	1028	1031	1037	rBV2	45062	98675	1.60%	0.233%
32	13.685	1039	1041	1044	rBV	1049099	1298971	21.04%	3.064%
33	15.045	1157	1160	1168	rBV	671723	892719	14.46%	2.106%
34	19.469	1539	1547	1548	rBV2	45406	154063	2.50%	0.363%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

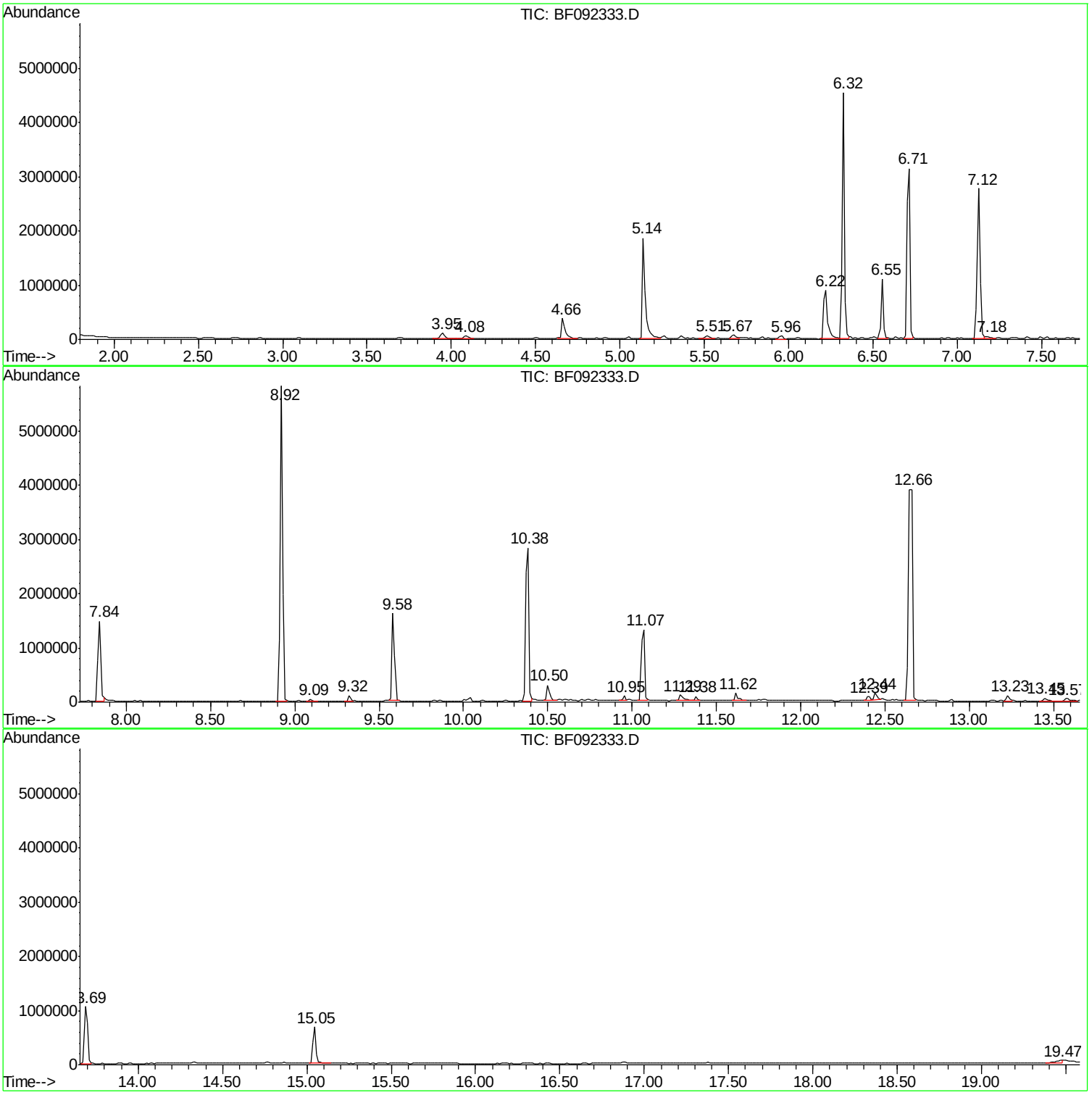
Sum of corrected areas: 42390243

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

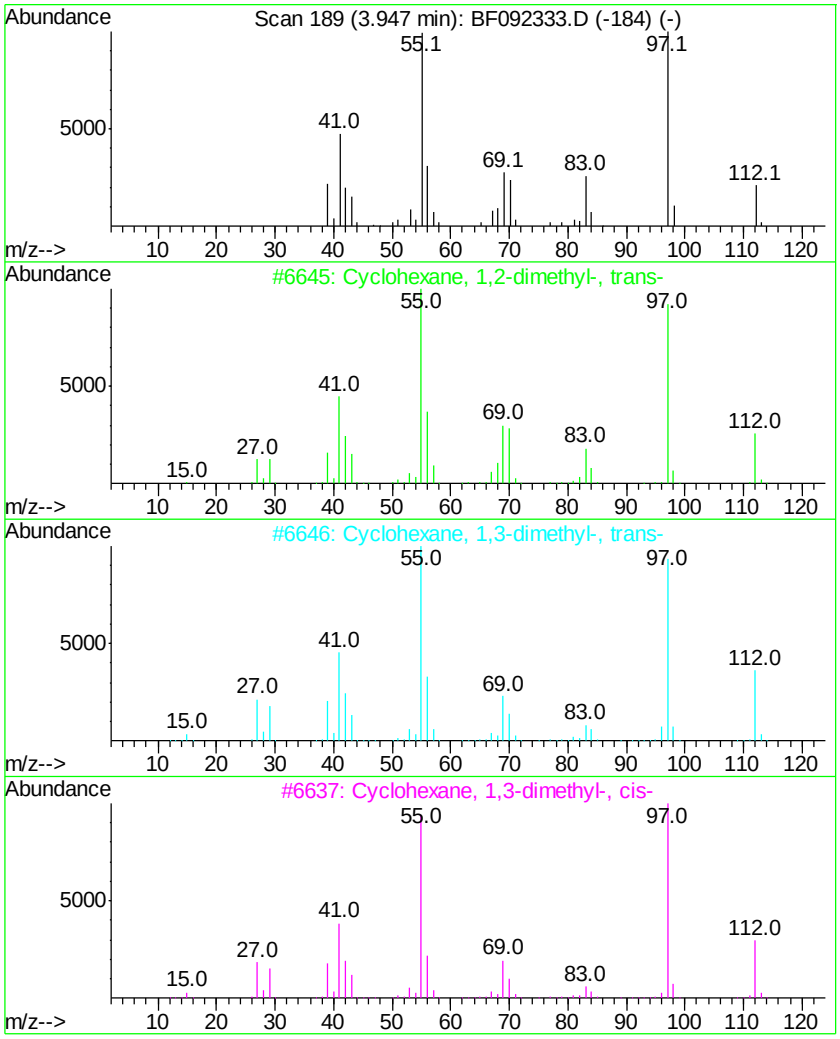
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

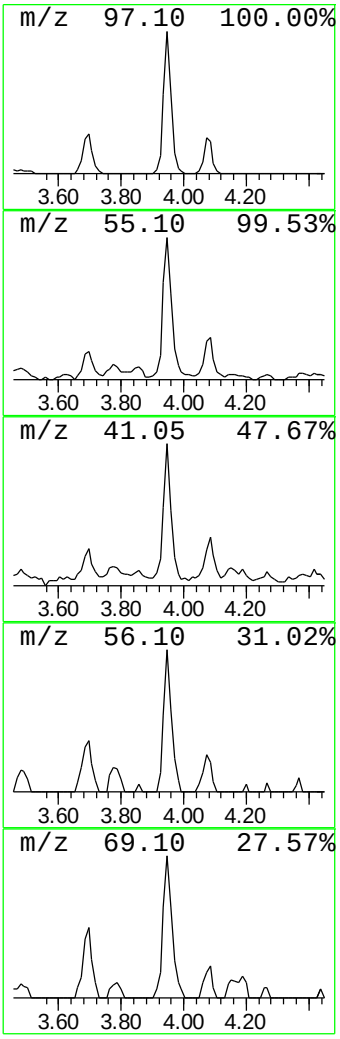
****

Peak Number 1 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	3.90 ng	197412	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	97
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	83
4	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	76
5	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

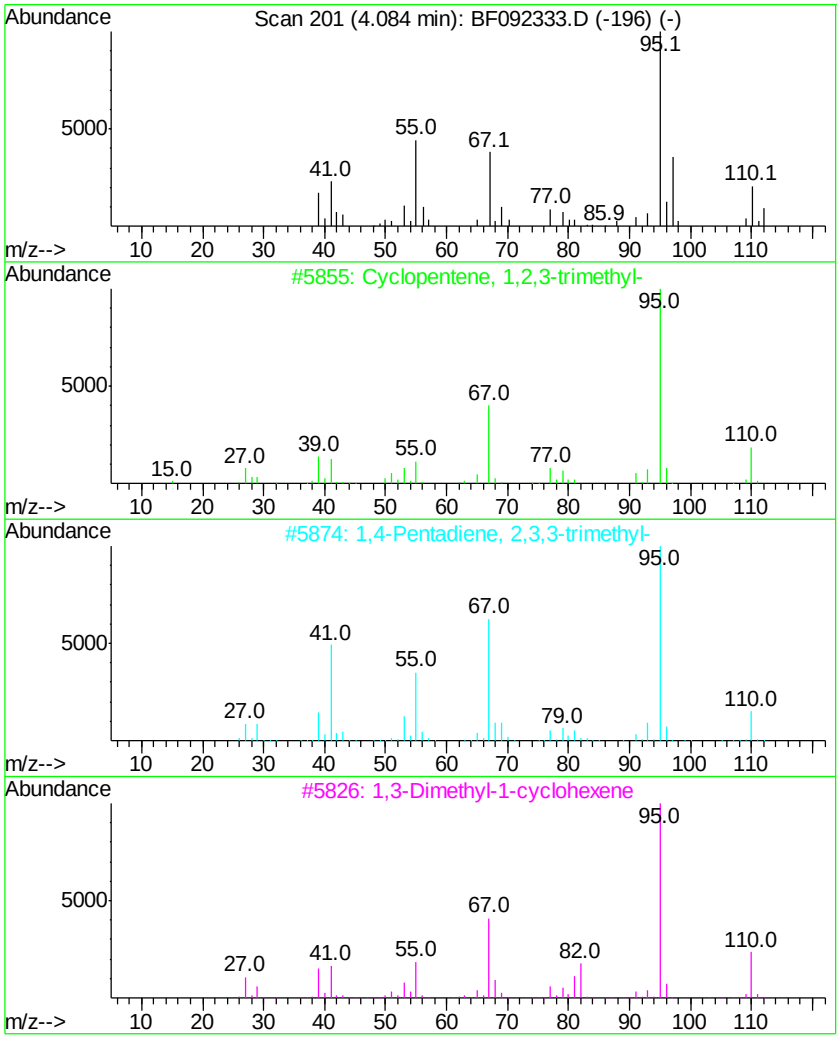
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

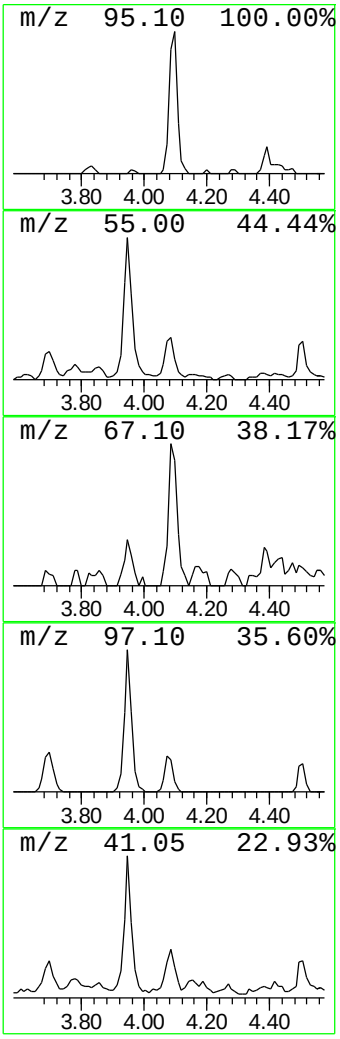
****

Peak Number 2 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	2.12 ng	107471	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	70
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	64
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	62
4	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	59
5	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	58





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

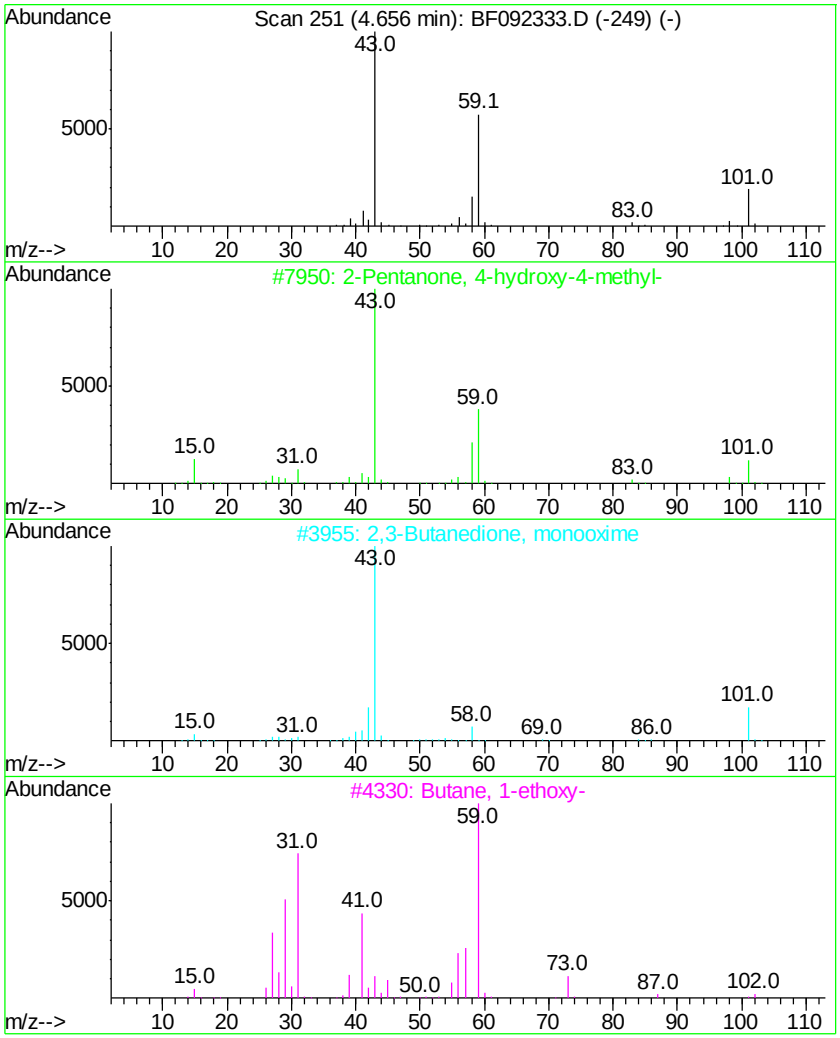
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

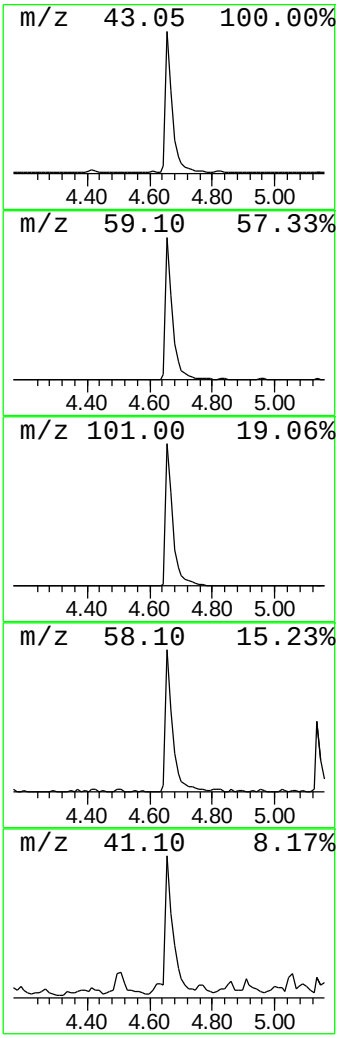
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	11.09 ng	561859	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

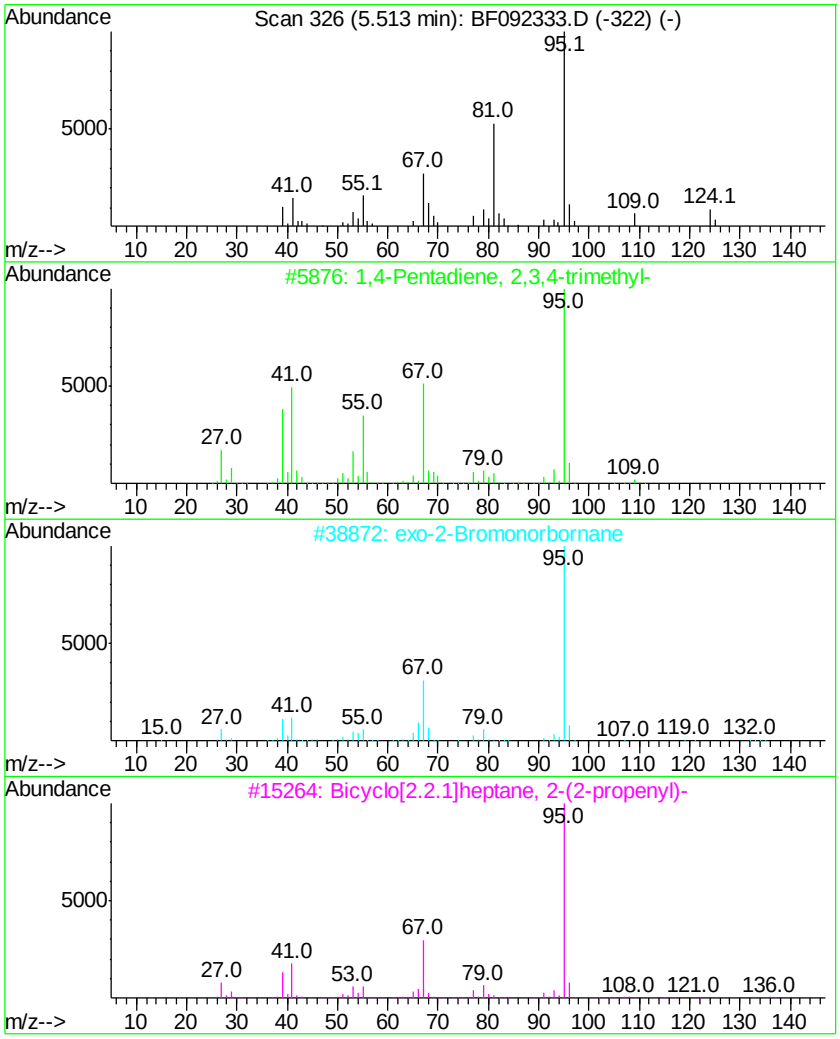
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

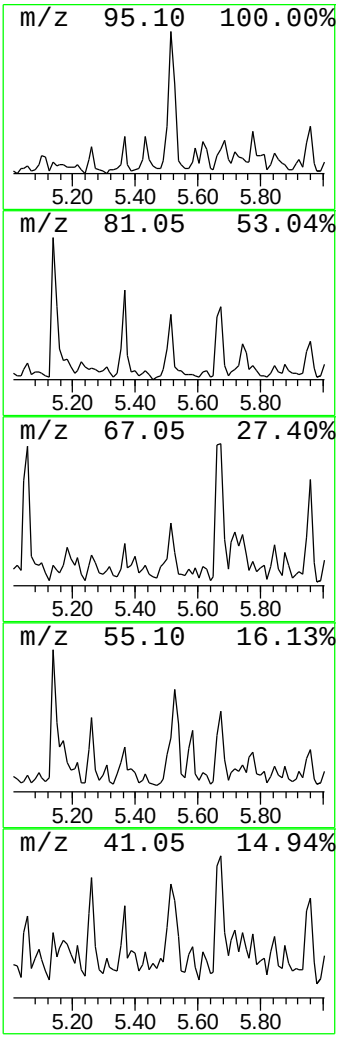
****

Peak Number 4 1,4-Pentadiene, 2,3,4-trime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	2.54 ng	128763	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	64
2	exo-2-Bromonorbornane	174	C7H11Br	002534-77-2	64
3	Bicyclo[2.2.1]heptane, 2-(2-prop...	136	C10H16	002633-80-9	59
4	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	59
5	2-Norbornyl bromide	174	C7H11Br	029342-65-2	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

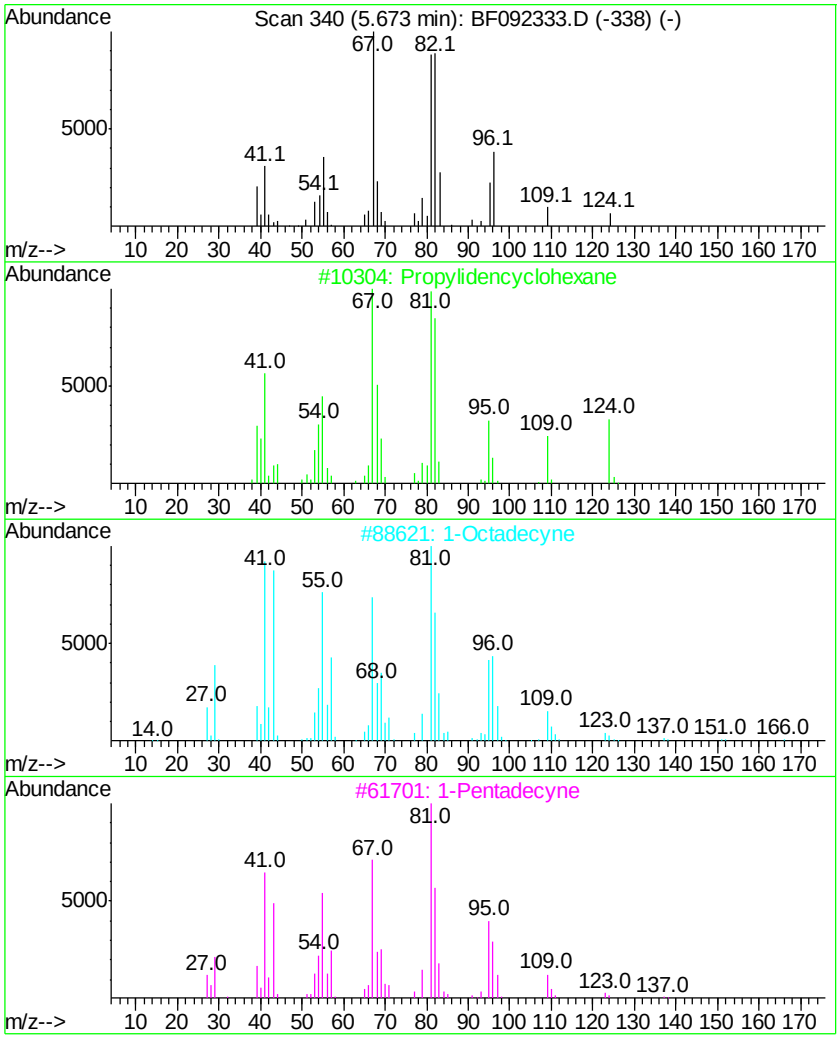
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

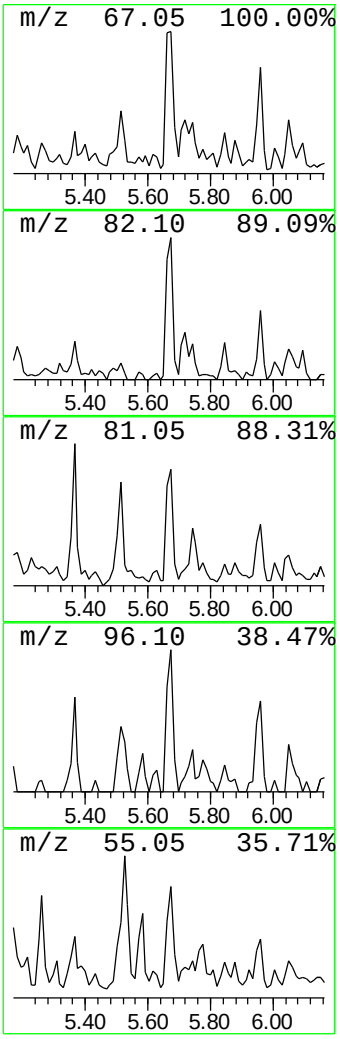
****

Peak Number 5 Propylidencyclohexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	2.91 ng	147508	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylidencyclohexane	124	C9H16	002129-93-3	64
2	1-Octadecyne	250	C18H34	000629-89-0	50
3	1-Pentadecyne	208	C15H28	000765-13-9	49
4	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	47
5	1-Heptadecyne	236	C17H32	026186-00-5	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

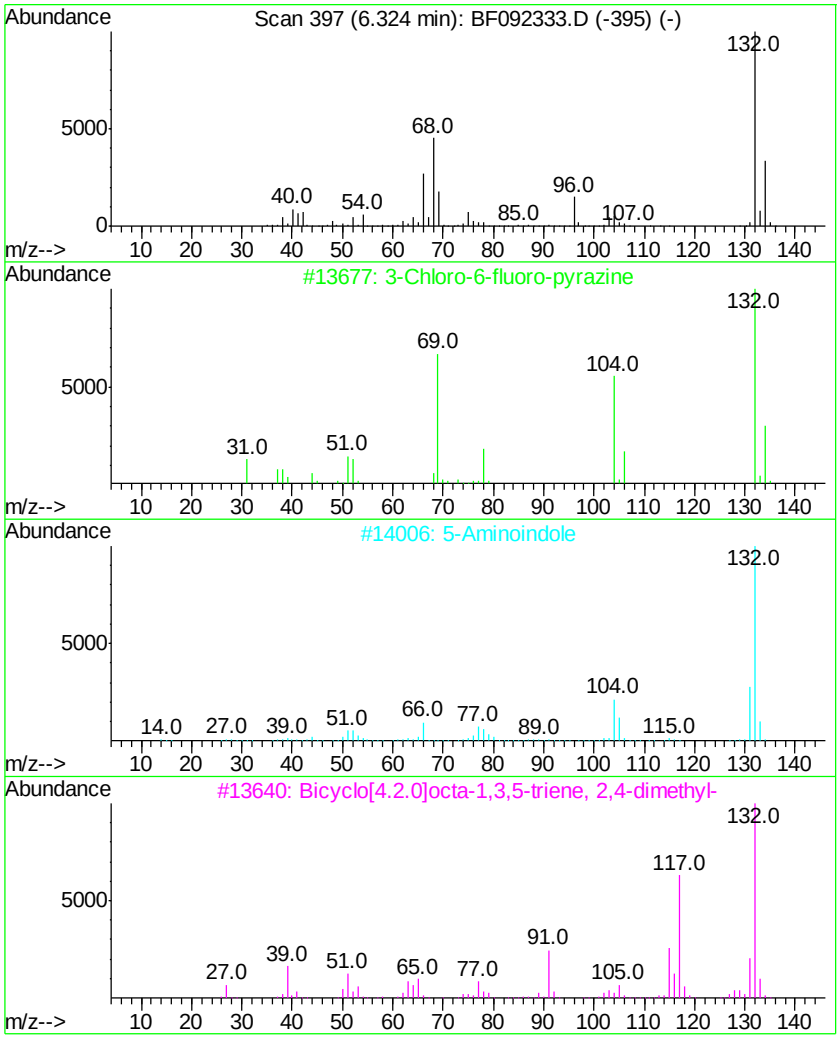
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

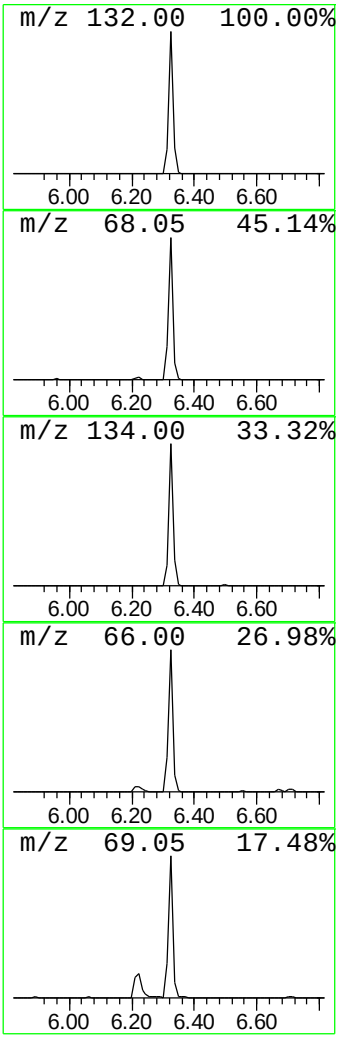
****

Peak Number 6 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	84.49 ng	4278920	1,4-Dichlorobenzene-d4	6.55

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

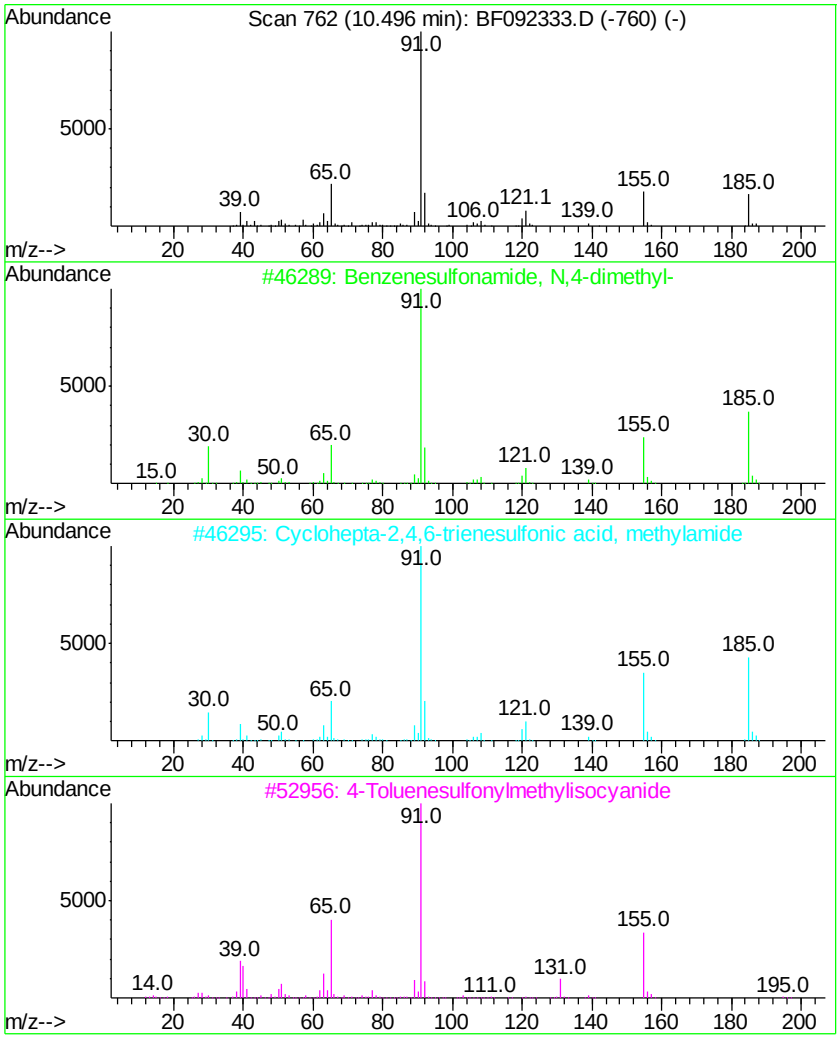
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

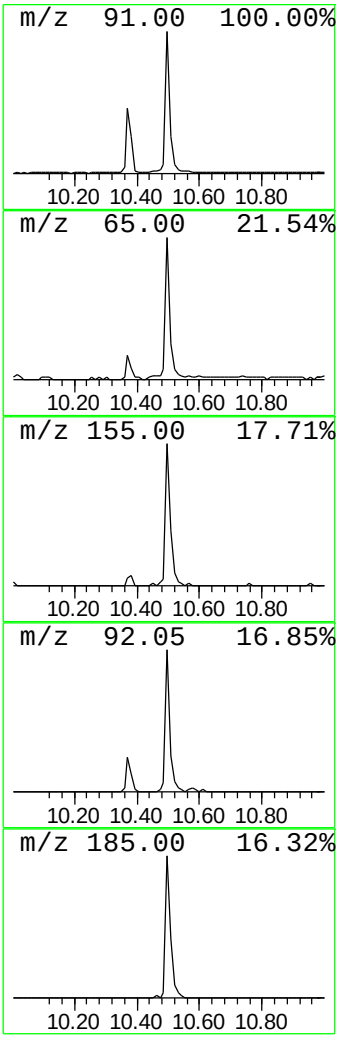
****

Peak Number 8 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	4.21 ng	361451	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	91
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	76
3	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	53
4	Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	53
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

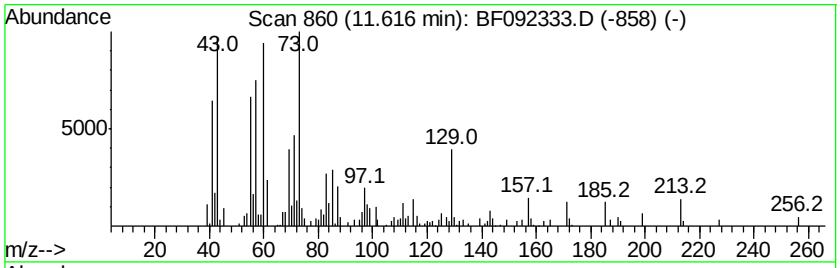
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

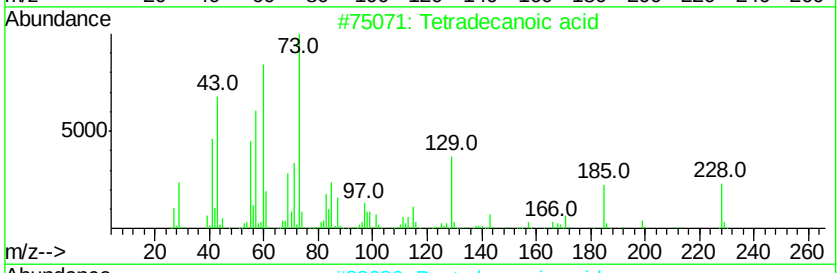
****

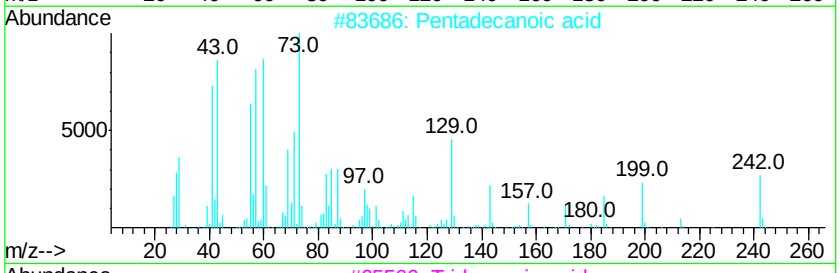
Peak Number 9 Tetradecanoic acid Concentration Rank 10

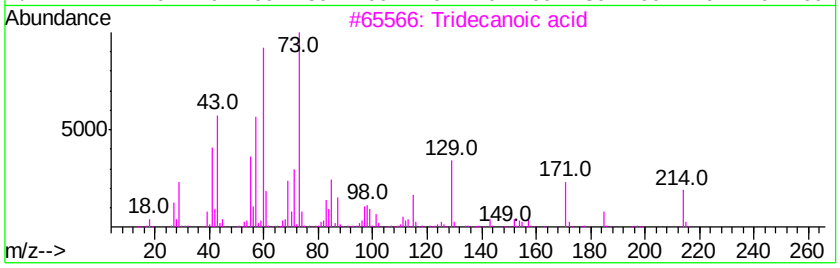
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.28 ng	195483	Phenanthrene-d10	11.07

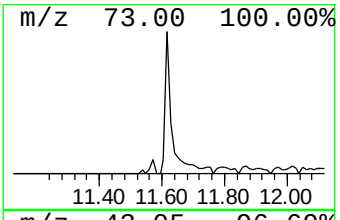
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53

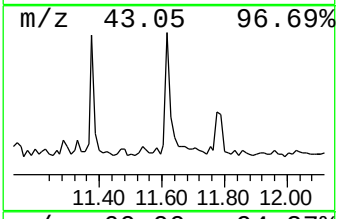


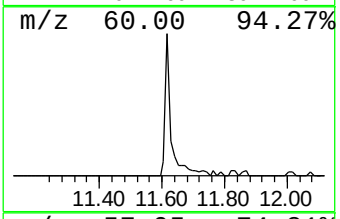


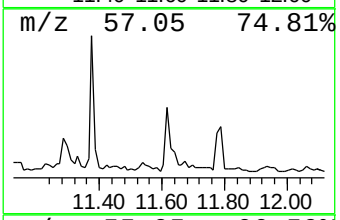


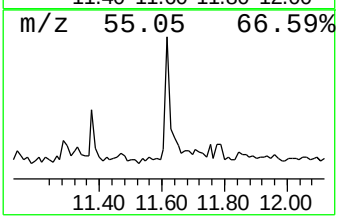












Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

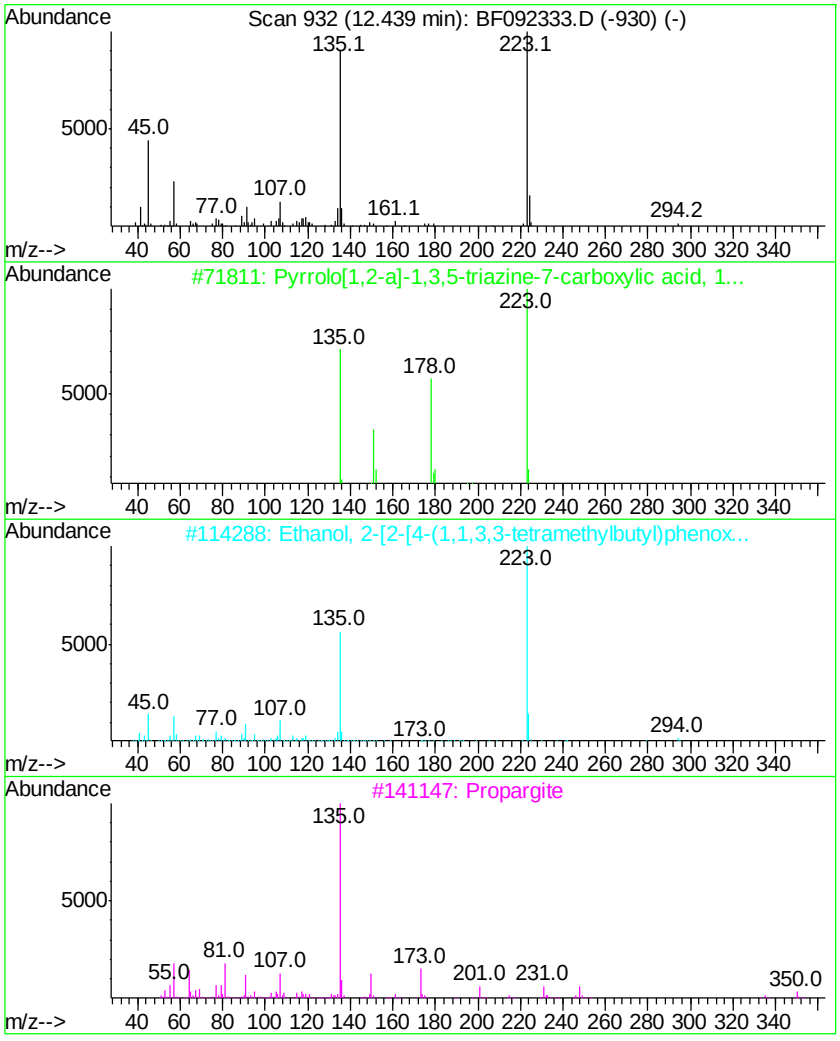
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

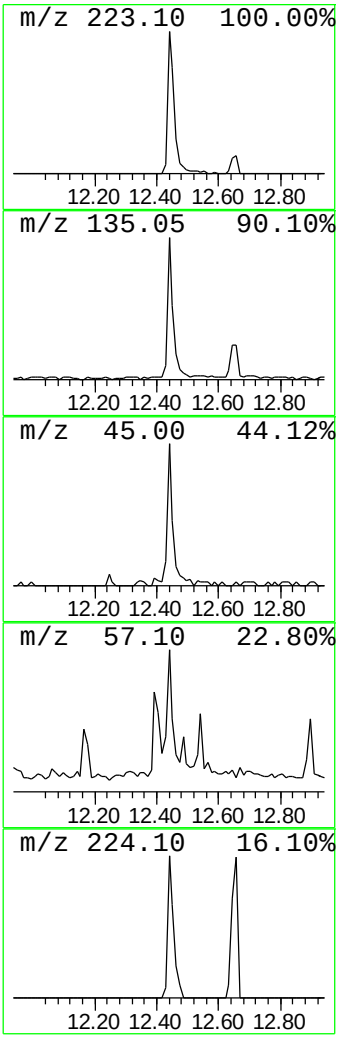
****

Peak Number 10 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	2.59 ng	167933	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	50
3	Propargite	350	C19H26O4S	002312-35-8	35
4	Ketoprofen di-methyl derivative	282	C18H18O3	1000137-08-9	35
5	1-n-butyladamantane	192	C14H24	014449-41-3	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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

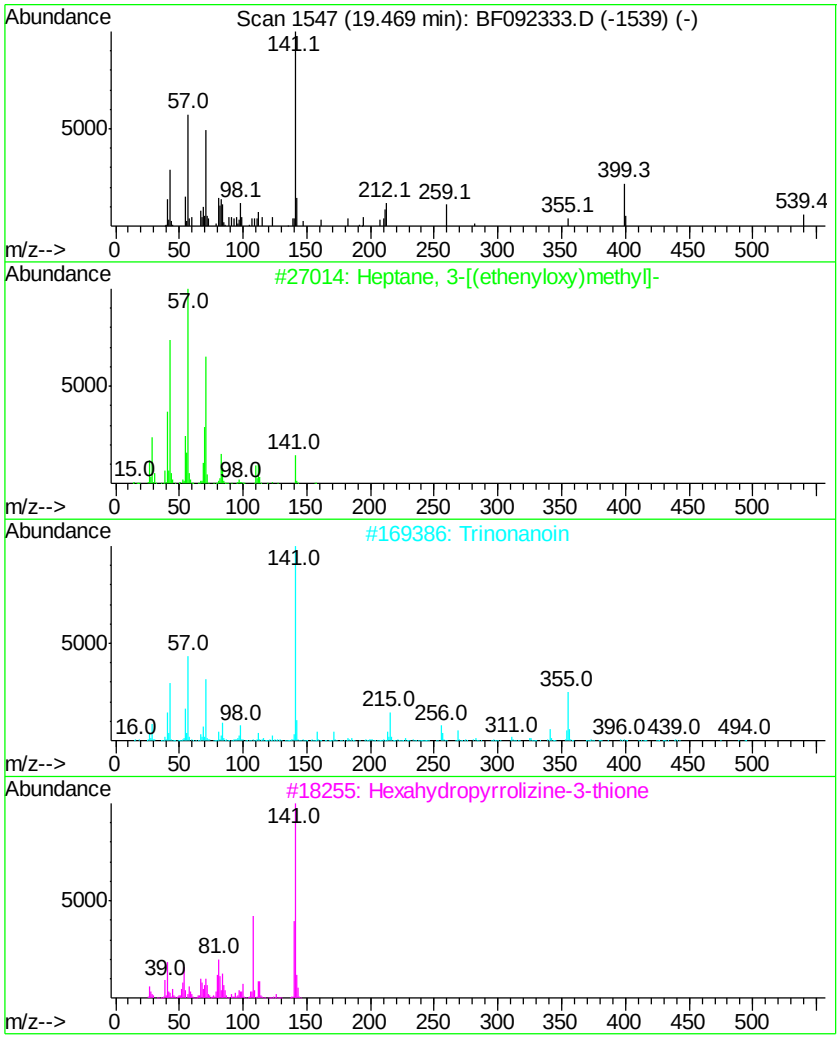
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

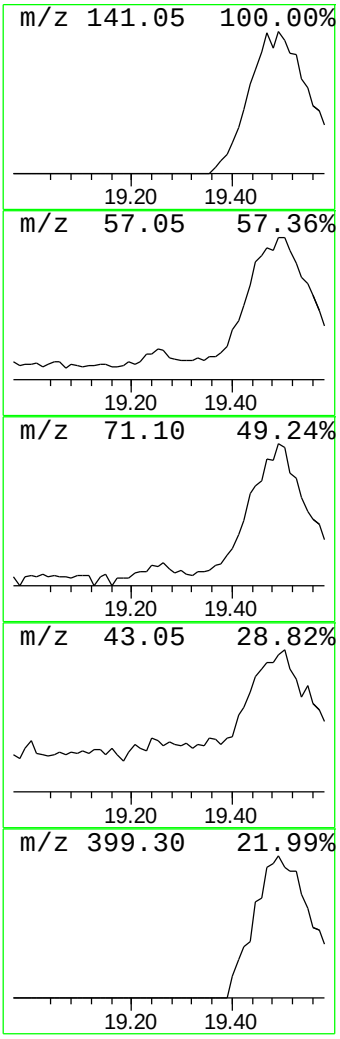
****

Peak Number 11 Heptane, 3-[(ethenyloxy)met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	3.45 ng	154063	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	50
2	Trinonanoin	512	C30H56O6	000126-53-4	37
3	Hexahydropyrrolizine-3-thione	141	C7H11NS	1000190-80-9	30
4	2-Fluorobenzoic acid, heptadecyl...	378	C24H39FO2	1000282-96-6	25
5	2H,7H-Pyrano[2,3-b]pyran, hexahy...	142	C8H14O2	038737-53-0	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011717\
Data File : BF092333.D
Acq On : 17 Jan 2017 23:21
Operator : UM/SJ
Sample : I1242-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-42

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
Cyclohexane, 1,2-...	3.95	3.9	ng	197412	1	6.55	1012840	20.0
Cyclopentene, 1,2...	4.08	2.1	ng	107471	1	6.55	1012840	20.0
2-Pentanone, 4-hy...	4.66	11.1	ng	561859	1	6.55	1012840	20.0
1,4-Pentadiene, 2...	5.51	2.5	ng	128763	1	6.55	1012840	20.0
Propylidencyclohe...	5.67	2.9	ng	147508	1	6.55	1012840	20.0
unknown6.32	6.32	84.5	ng	4278920	1	6.55	1012840	20.0
Benzenesulfonamid...	10.50	4.2	ng	361451	4	11.07	1716820	20.0
Tetradecanoic acid	11.62	2.3	ng	195483	4	11.07	1716820	20.0
Pyrrolo[1,2-a]-1,...	12.44	2.6	ng	167933	5	13.69	1298970	20.0
Heptane, 3-[(ethe...	19.47	3.5	ng	154063	6	15.05	892719	20.0