LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022519\
Data File : BF112702.D
Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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	6.616	766	770	772	rBV	340687	286778	1.62%	0.687%
2	6.645	772	775	779	rVB	320926	286141	1.62%	0.686%
3	6.739	787	791	801	rBV	378813	397202	2.25%	0.952%
4	6.816	801	804	814	rBV	347020	348742	1.98%	0.836%
5	7.728	952	959	963	rBV	141089	189539	1.07%	0.454%
6	7.833	971	977	984	rBV2	331905	435512	2.47%	1.044%
7	7.898	984	988	990	rBV2	164819	217395	1.23%	0.521%
8	7.933	990	994	995	rVV	365722	407840	2.31%	0.978%
9	7.986	998	1003	1007	rVV6	931466	1985591	11.25%	4.759%
10	8.033	1007	1011	1018	rVV3	1102222	2670093	15.12%	6.400%
11	8.092	1018	1021	1027	rVB2	1507518	1617128	9.16%	3.876%
12	8.157	1027	1032	1033	rBV3	349925	528449	2.99%	1.267%
13	8.186	1033	1037	1041	rVB2	864305	1107441	6.27%	2.654%
14	8.257	1044	1049	1053	rBV3	603393	961261	5.44%	2.304%
15	8.522	1091	1094	1107	rVB	1278332	1352617	7.66%	3.242%
16	9.680	1281	1291	1294	rBV	10501514	17657218	100.00%	42.323%
17	9.851	1317	1320	1326	rVB	493308	437264	2.48%	1.048%
18	10.663	1452	1458	1469	rBV	6711492	7473455	42.33%	17.913%
19	11.339	1570	1573	1583	rVB	396072	382916	2.17%	0.918%
20	11.545	1605	1608	1621	rBV	1520058	1597296	9.05%	3.829%
21	13.809	1988	1993	2001	rBV	158854	224779	1.27%	0.539%
22	13.980	2020	2022	2031	rVB	442416	496494	2.81%	1.190%
23	14.939	2181	2185	2194	rVV	234881	302932	1.72%	0.726%
24	15.456	2268	2273	2282	rBV	254372	355751	2.01%	0.853%

Sum of corrected areas: 41719834

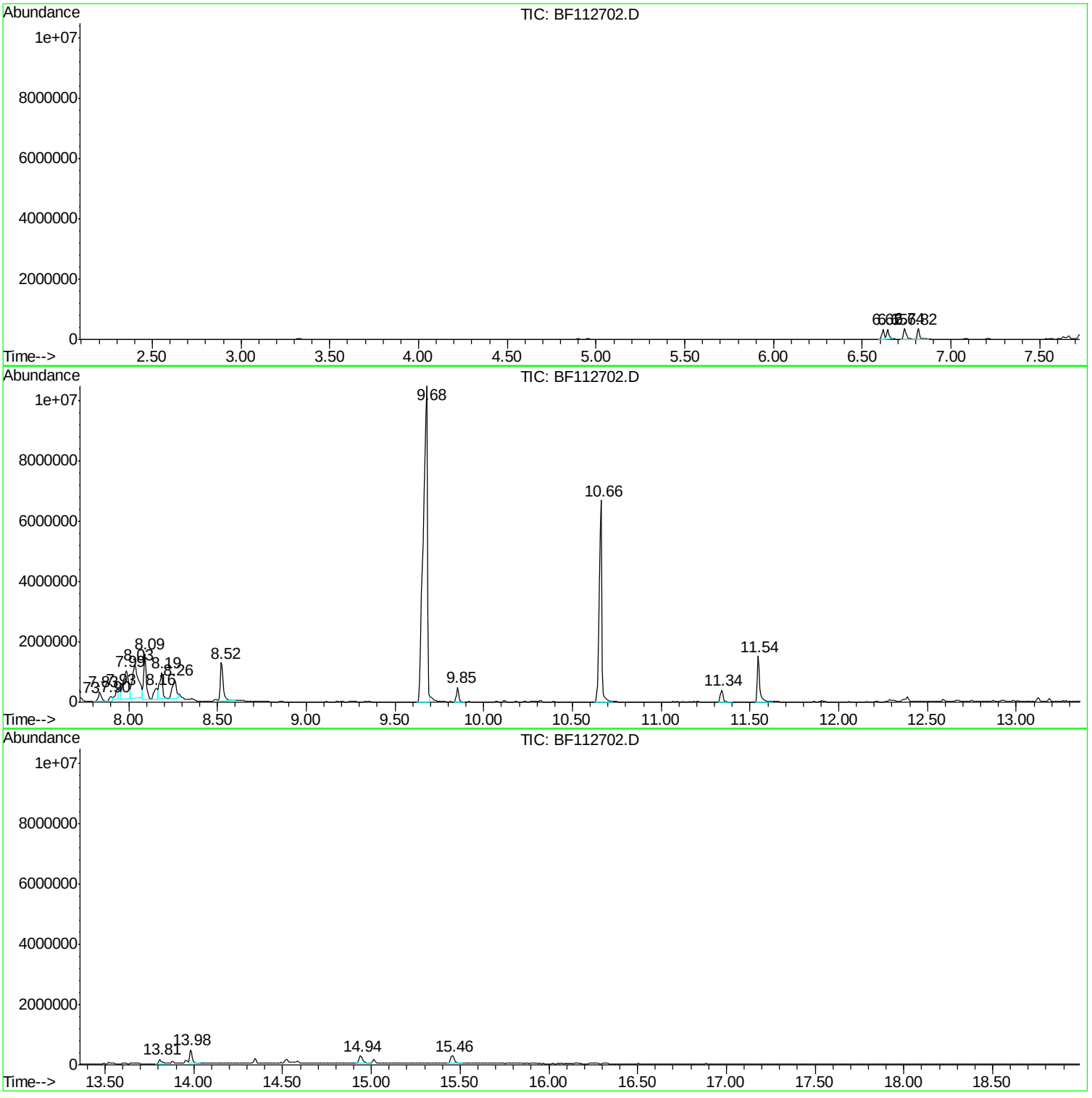
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022519\
Data File : BF112702.D
Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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

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Data File : BF112702.D
Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

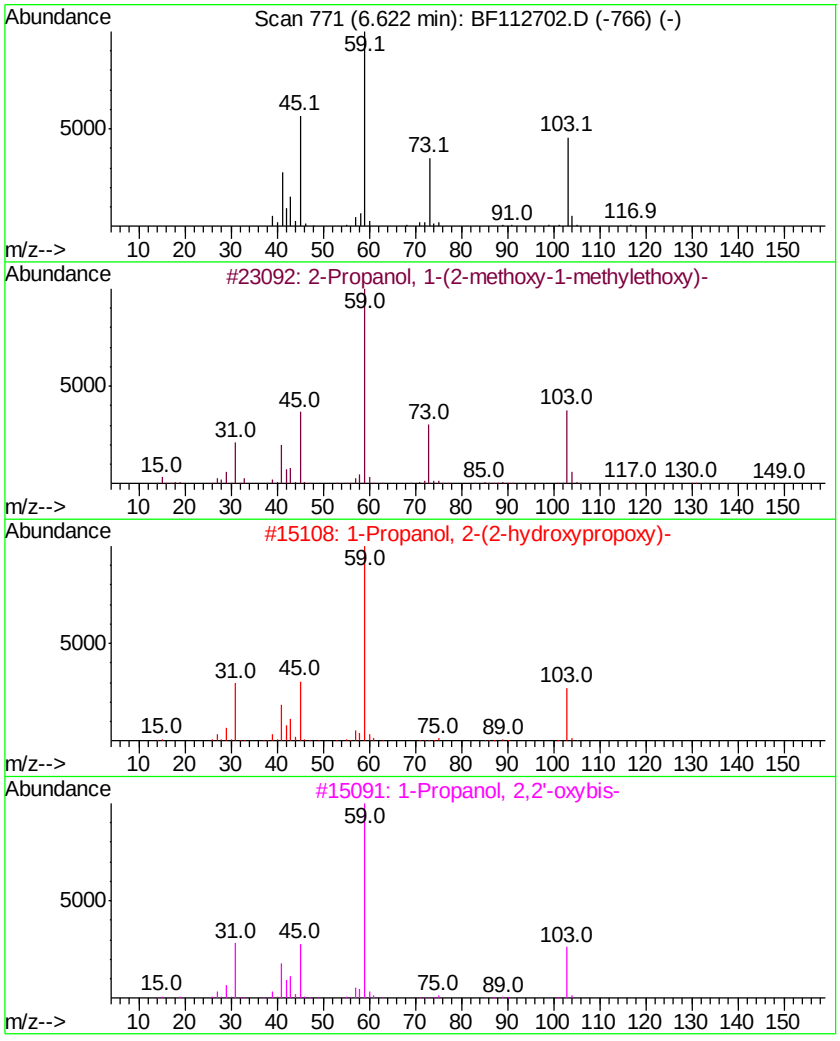
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

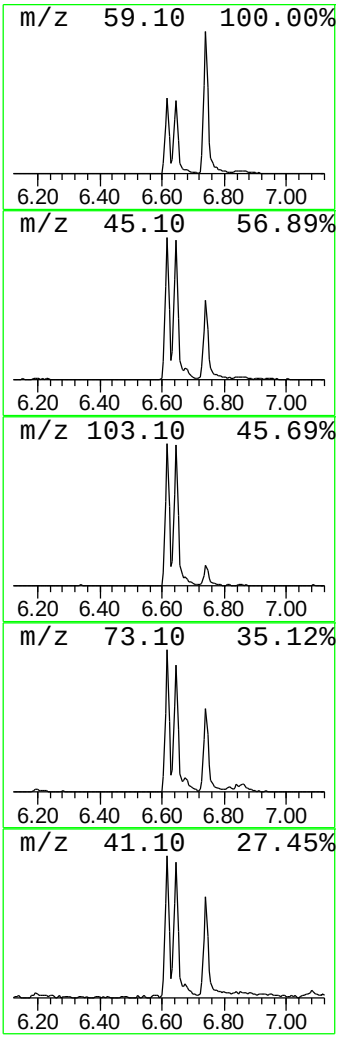
****

Peak Number 1 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	16.45 ng	286778	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	86
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	45
5	2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	42





Library Search Compound Report

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Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

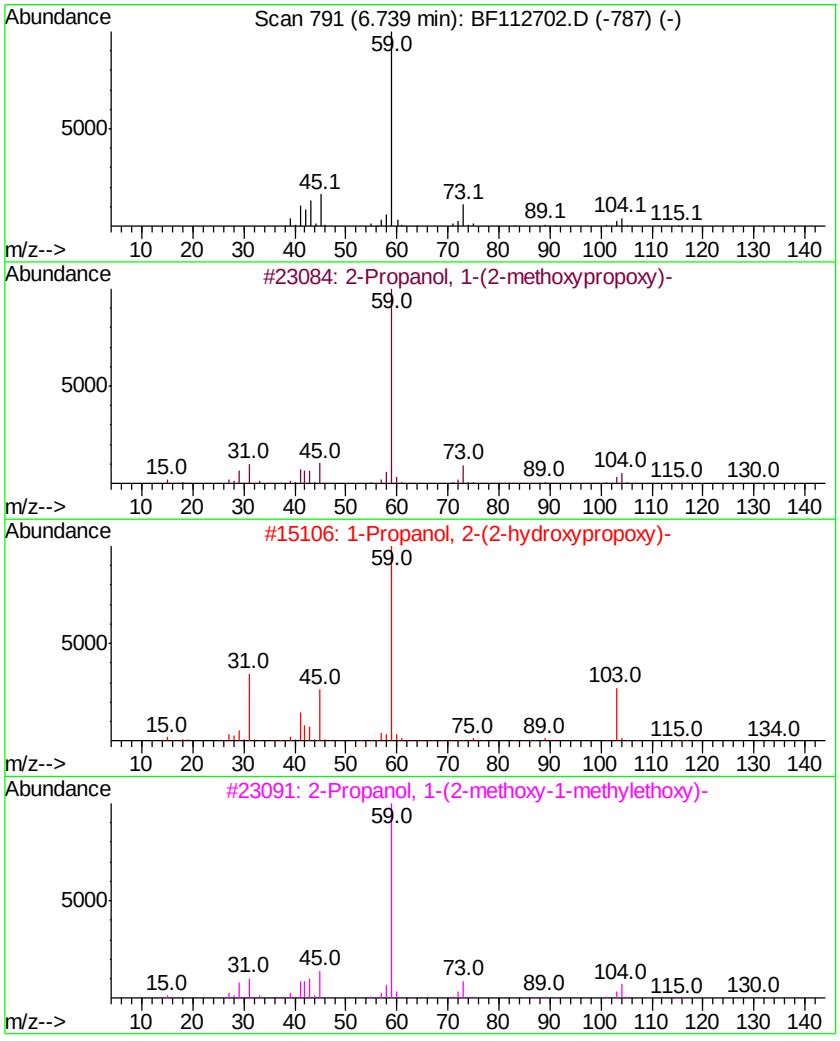
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

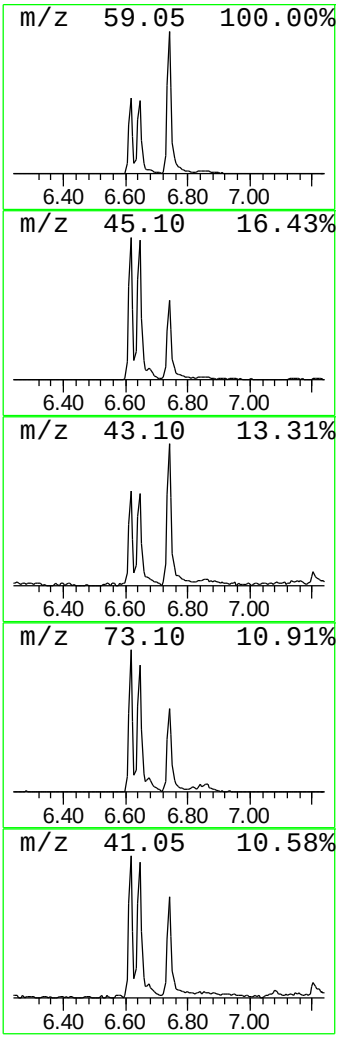
****

Peak Number 3 2-Propanol, 1-(2-methoxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	22.78 ng	397202	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	50
4	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	50
5	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	50





Library Search Compound Report

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Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
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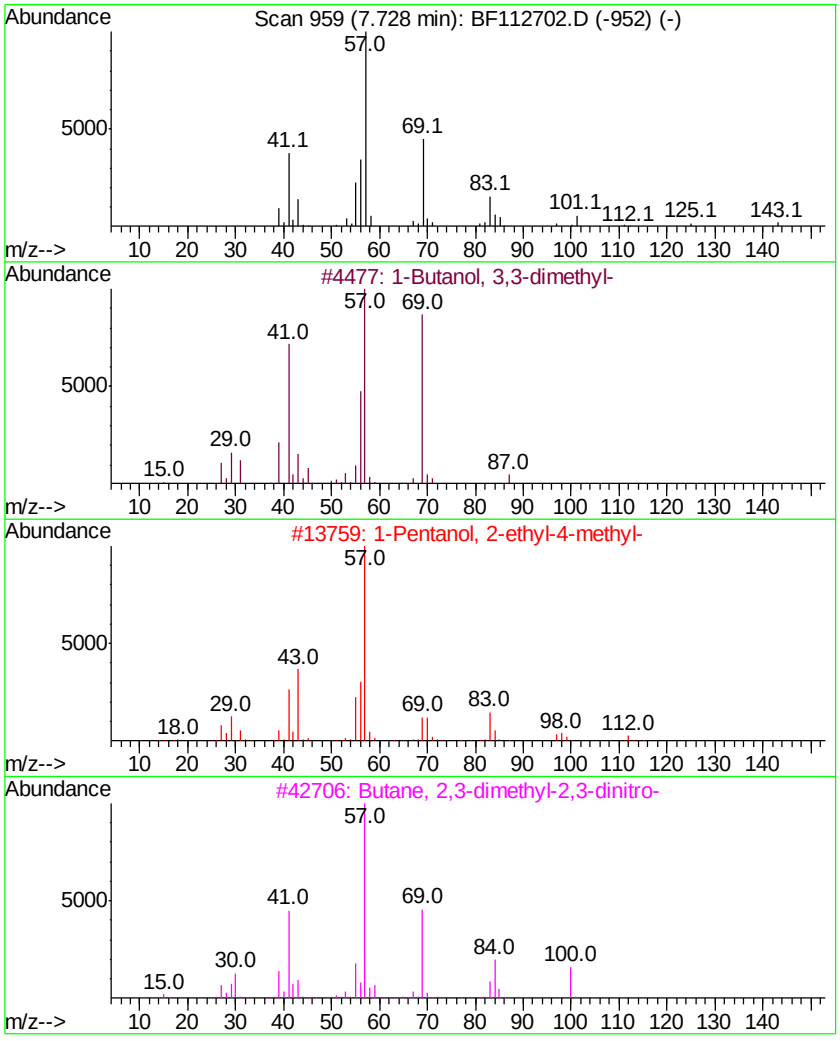
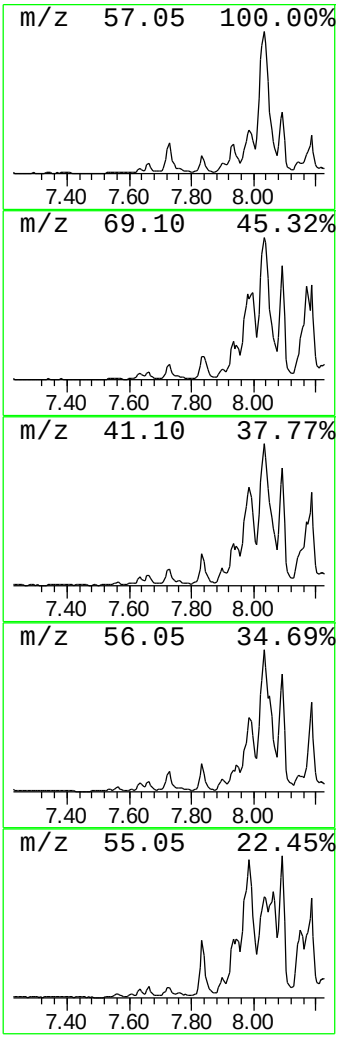
****

Peak Number 4 unknown7.73 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	2.34 ng	189539	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	47
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	39
3	Butane, 2,3-dimethyl-2,3-dinitro-	176	C6H12N2O4	003964-18-9	38
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	38
5	Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	38





Library Search Compound Report

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Data File : BF112702.D
Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

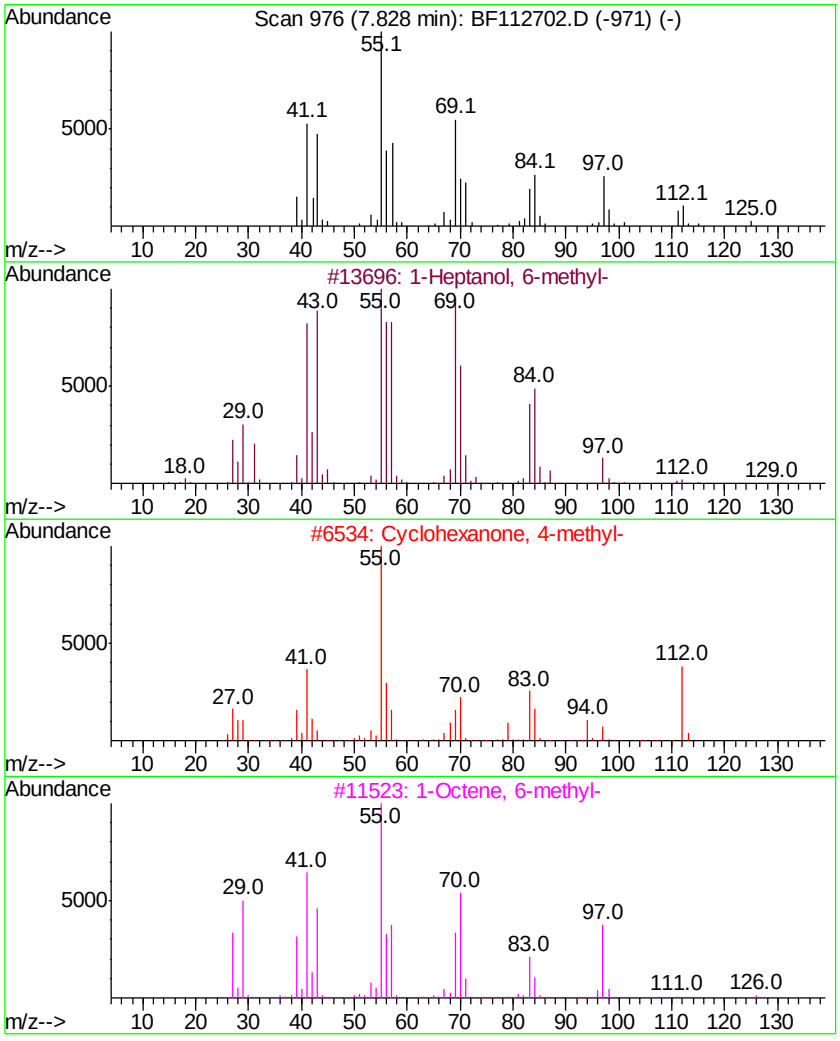
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

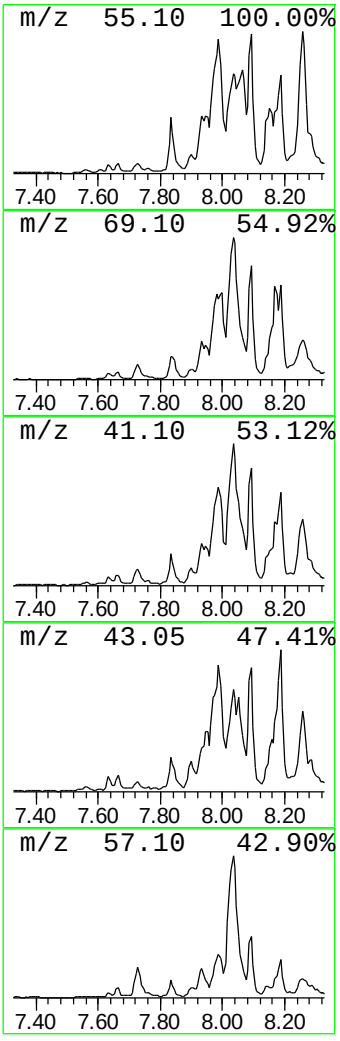
****

Peak Number 5 unknown7.83 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.83	5.39 ng	435512	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	47
2	Cyclohexanone, 4-methyl-	112	C7H12O	000589-92-4	47
3	1-Octene, 6-methyl-	126	C9H18	013151-10-5	47
4	1-Dodecene	168	C12H24	000112-41-4	43
5	4-Octene, (E)-	112	C8H16	014850-23-8	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022519\
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Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

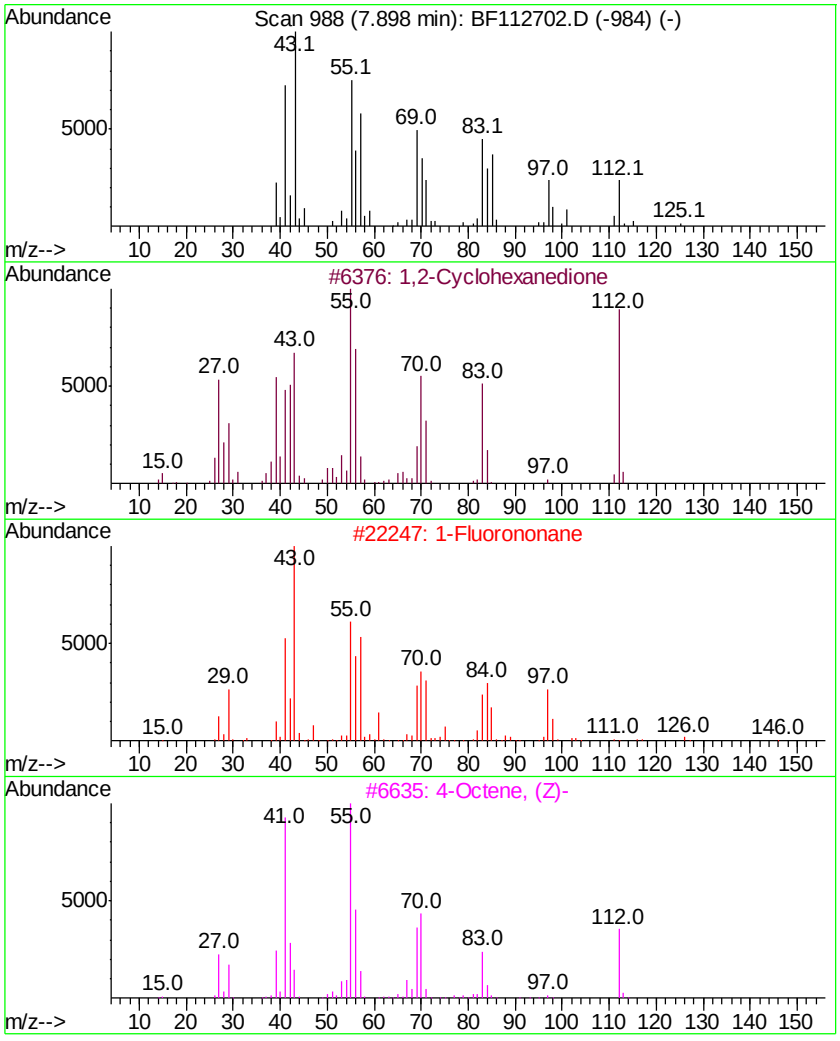
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

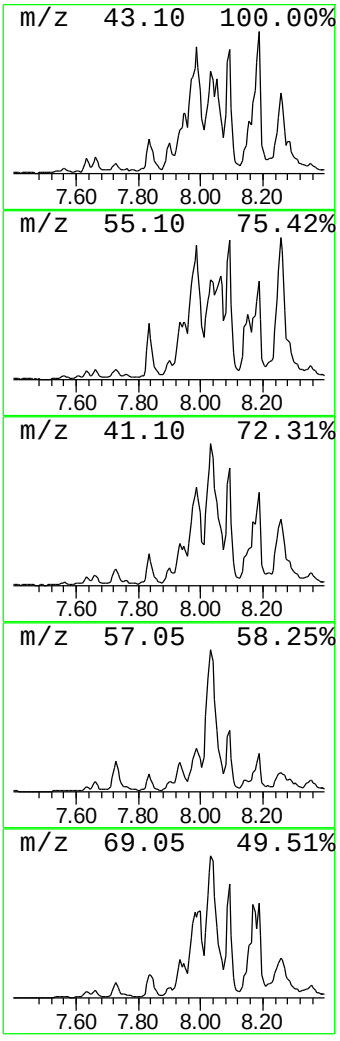
****

Peak Number 6 1,2-Cyclohexanedione Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.90	2.69 ng	217395	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	62
2	1-Fluorononane	146	C9H19F	000463-18-3	50
3	4-Octene, (Z)-	112	C8H16	007642-15-1	43
4	2-Octene, (Z)-	112	C8H16	007642-04-8	43
5	4-Pentenal, 2-ethyl-	112	C7H12O	005204-80-8	43





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Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

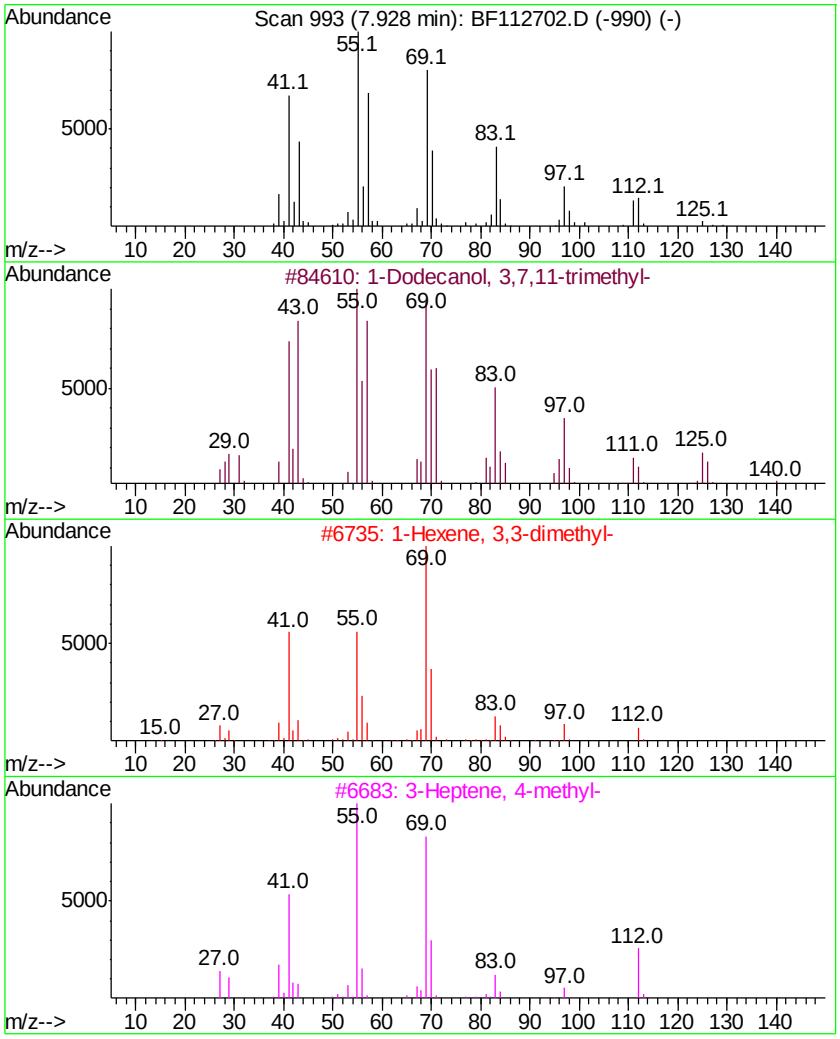
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

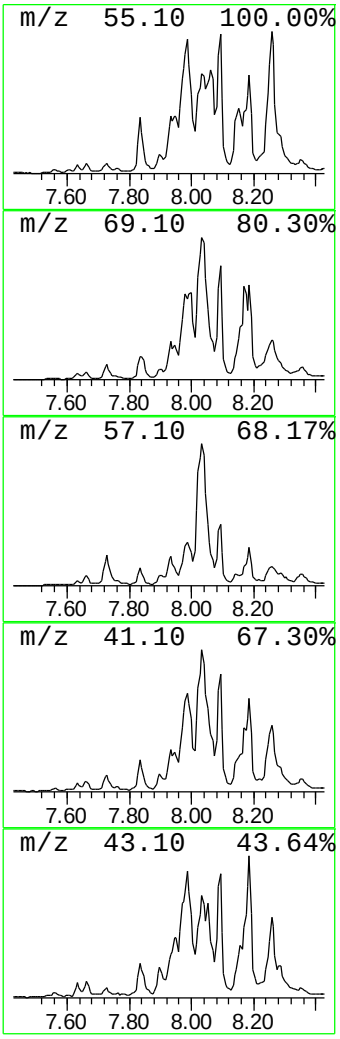
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Dodecanol, 3,7,11-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	5.04 ng	407840	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	80
2	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	68
3	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	58
4	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	49
5	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	46





Library Search Compound Report

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

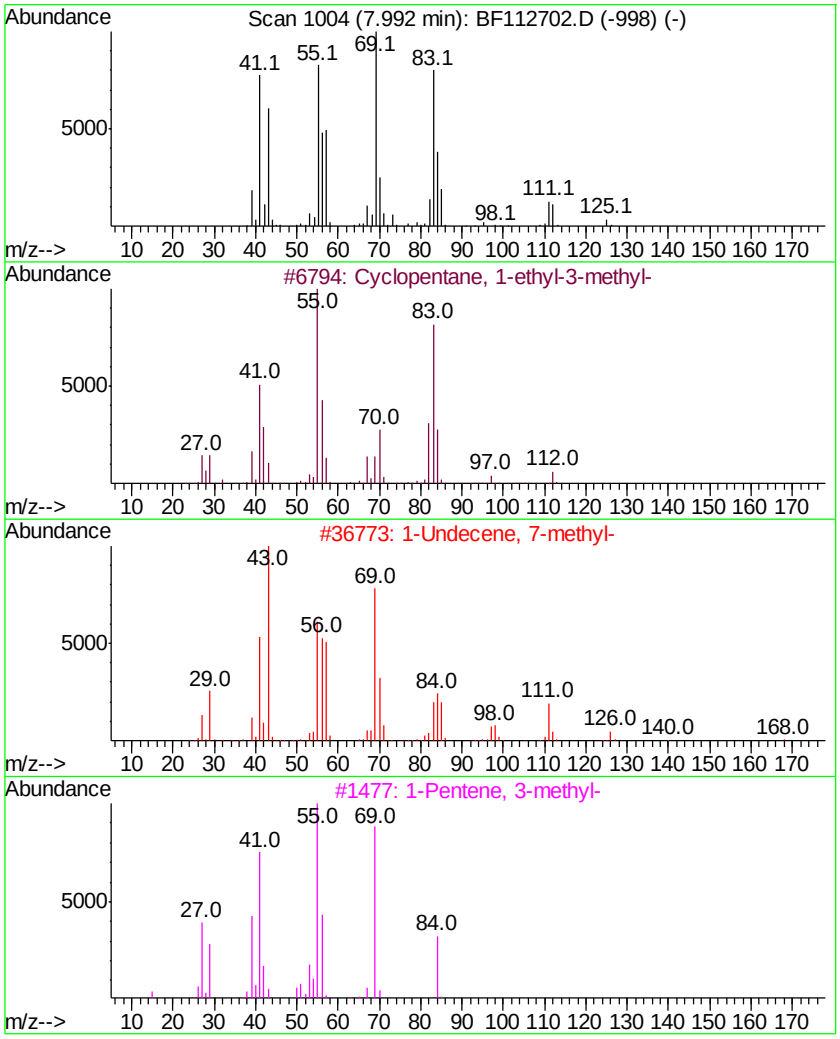
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

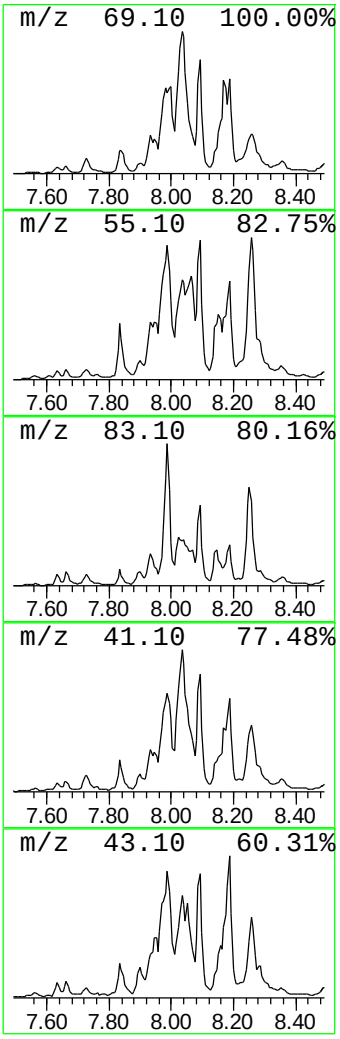
****

Peak Number 8 Cyclopentane, 1-ethyl-3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.99	24.56 ng	1985590	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	50
2	1-Undecene, 7-methyl-	168	C12H24	074630-42-5	47
3	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	43
4	Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-66-3	43
5	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	43





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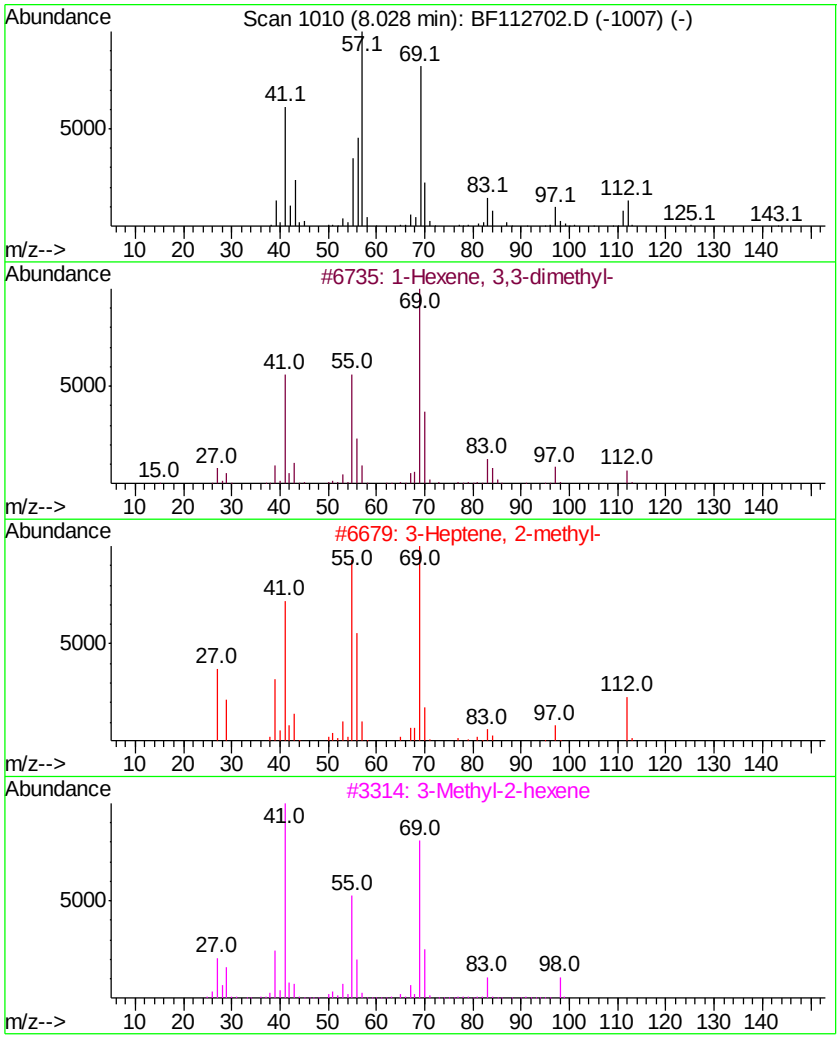
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

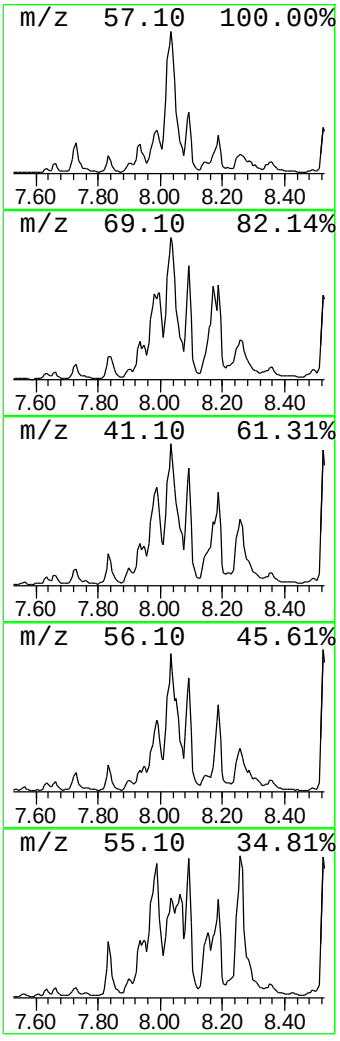
****

Peak Number 9 1-Hexene, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.03	33.02 ng	2670090	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	76
2	3-Heptene, 2-methyl-	112	C8H16	017618-76-7	53
3	3-Methyl-2-hexene	98	C7H14	017618-77-8	49
4	2-Methyl-2-heptene	112	C8H16	000627-97-4	49
5	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	43





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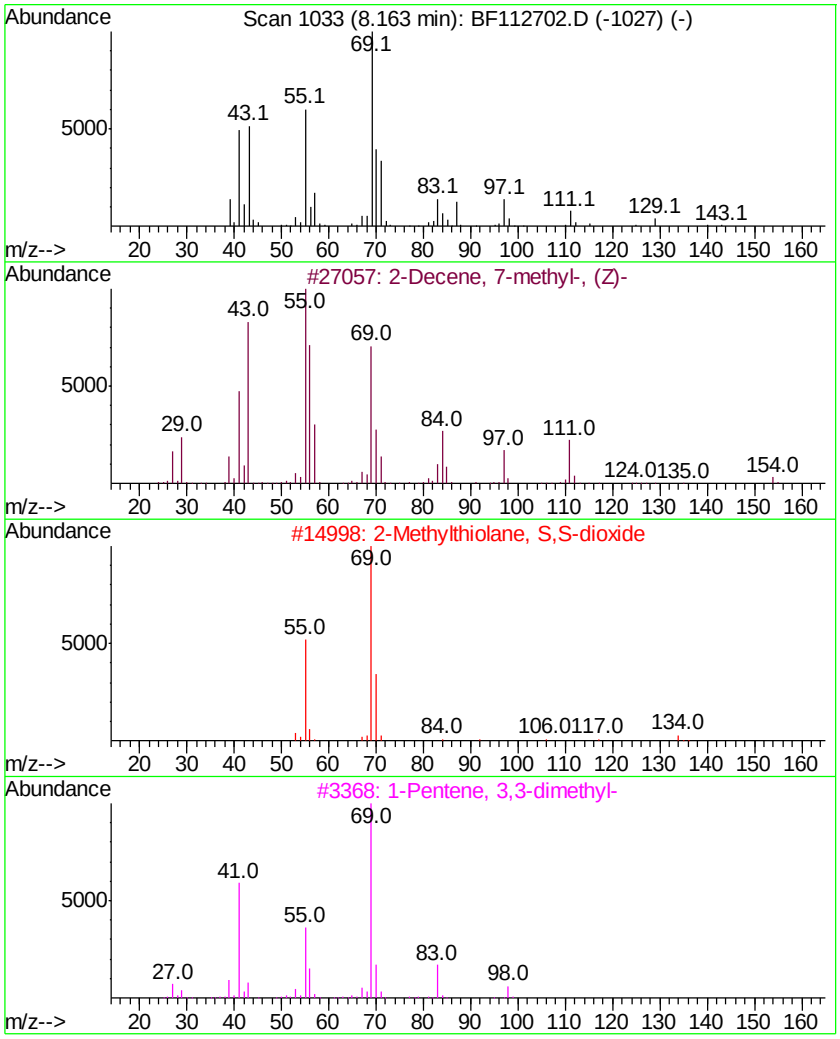
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

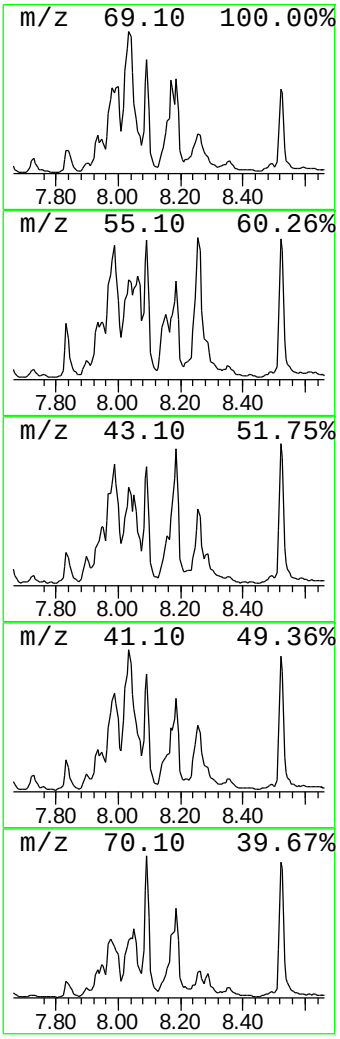
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Decene, 7-methyl-, (Z)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	6.54 ng	528449	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decene, 7-methyl-, (Z)-	154	C11H22	074630-23-2	53
2	2-Methylthiolane, S,S-dioxide	134	C5H10O2S	001003-46-9	43
3	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	43
4	Cyclohexane, 1-ethyl-1,4-dimethy...	140	C10H20	062238-32-8	43
5	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	42





Library Search Compound Report

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Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
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Misc :
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TIC Integration Parameters: LSCINT.P

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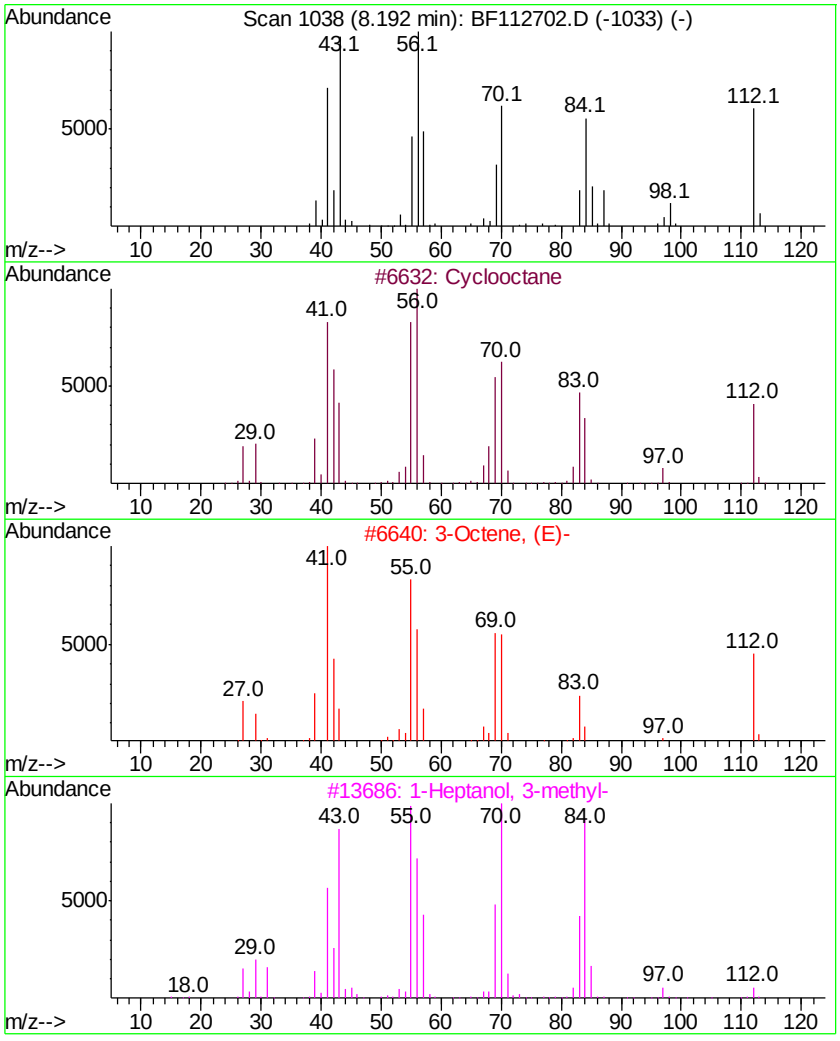
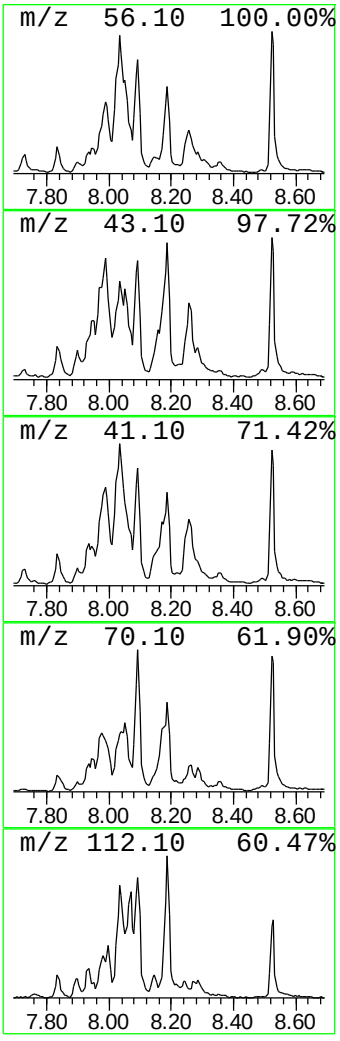
Peak Number 11 Cyclooctane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.19	13.70 ng	1107440	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane	112	C8H16	000292-64-8	64
2	3-Octene, (E)-	112	C8H16	014919-01-8	60
3	1-Heptanol, 3-methyl-	130	C8H18O	001070-32-2	59
4	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	52
5	Heptane, 4-methylene-	112	C8H16	015918-08-8	49





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Data File : BF112702.D
Acq On : 25 Feb 2019 19:40
Operator : JU/SJ
Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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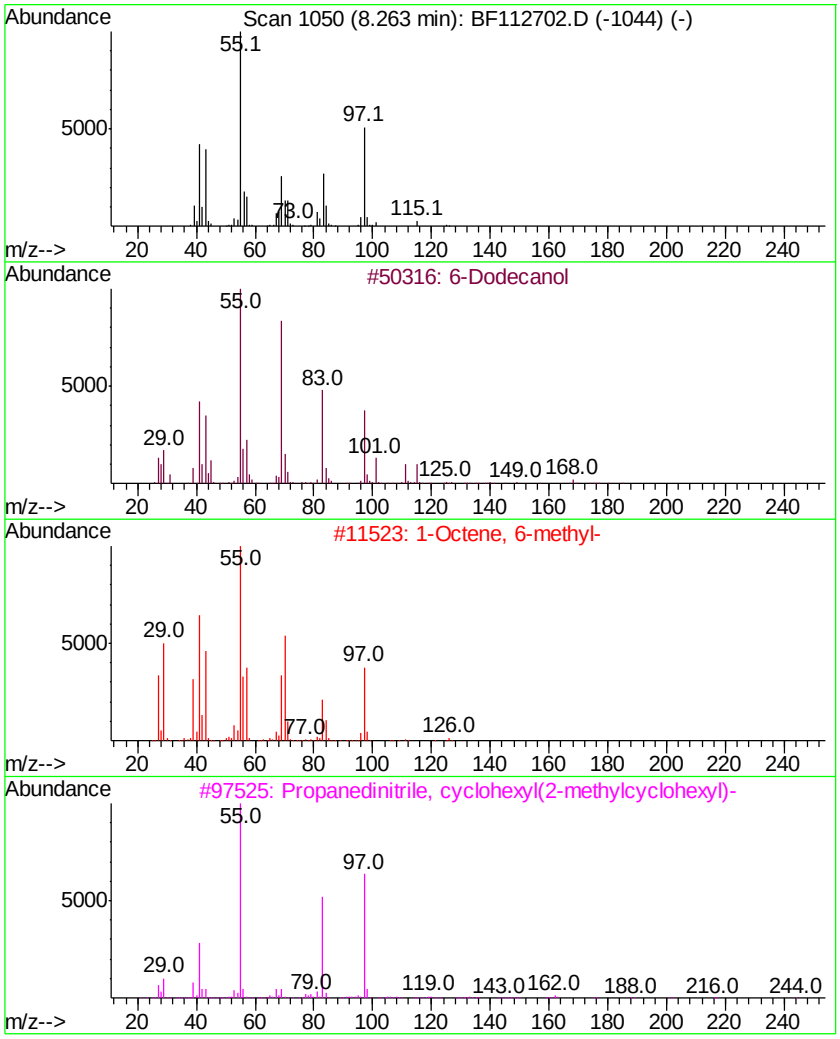
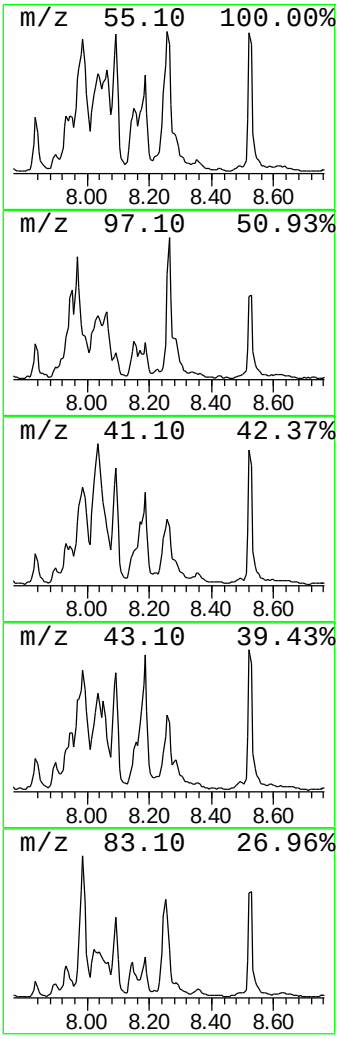
Peak Number 12 6-Dodecanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	11.89 ng	961261	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Dodecanol	186	C12H26O	006836-38-0	50
2	1-Octene, 6-methyl-	126	C9H18	013151-10-5	50
3	Propanedinitrile, cyclohexyl(2-m...	244	C16H24N2	074764-55-9	47
4	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	43
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	38





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

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TIC Library : C:\DATABASE\NIST11.L
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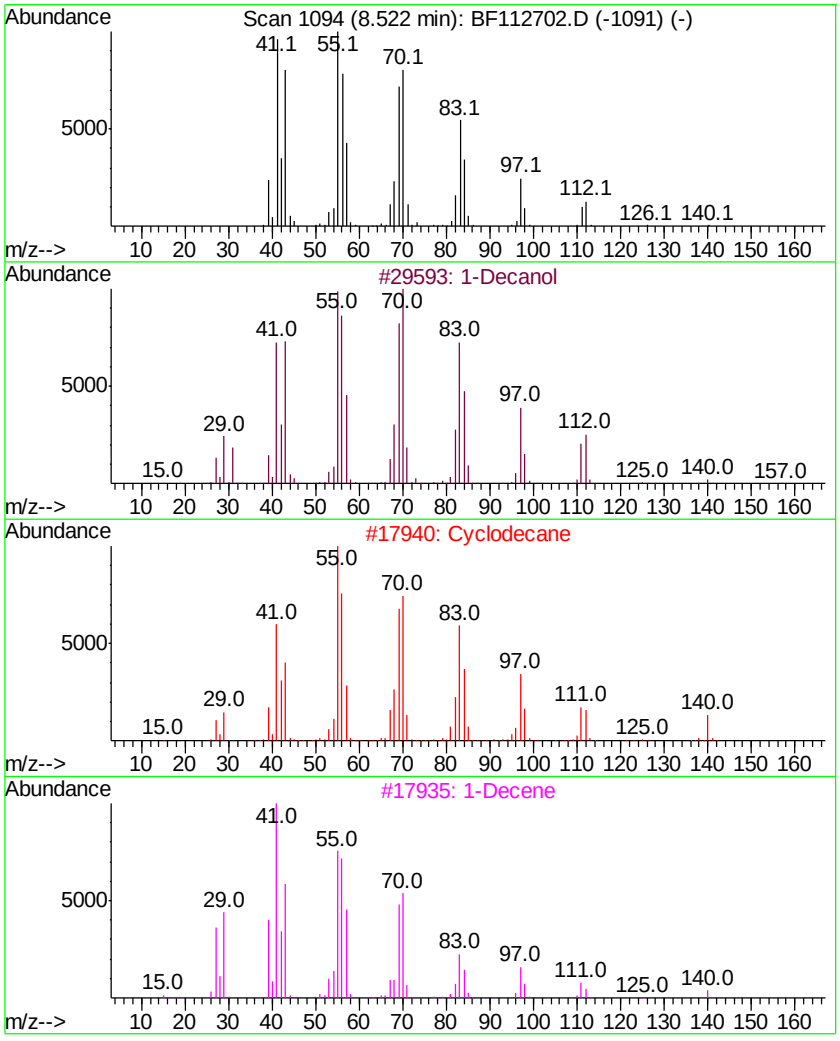
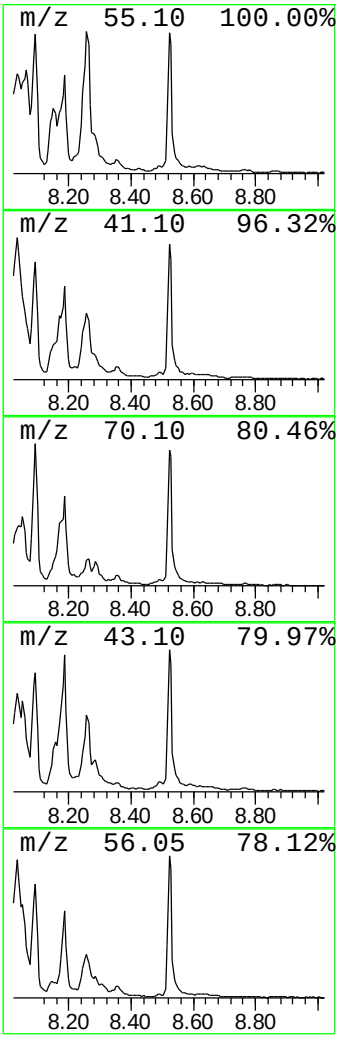
Peak Number 13 1-Decanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	16.73 ng	1352620	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	Cyclodecane	140	C10H20	000293-96-9	91
3	1-Decene	140	C10H20	000872-05-9	81
4	Cyclooctane	112	C8H16	000292-64-8	76
5	Octane, 2-chloro-	148	C8H17Cl	000628-61-5	72





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Sample : K1549-04 50X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

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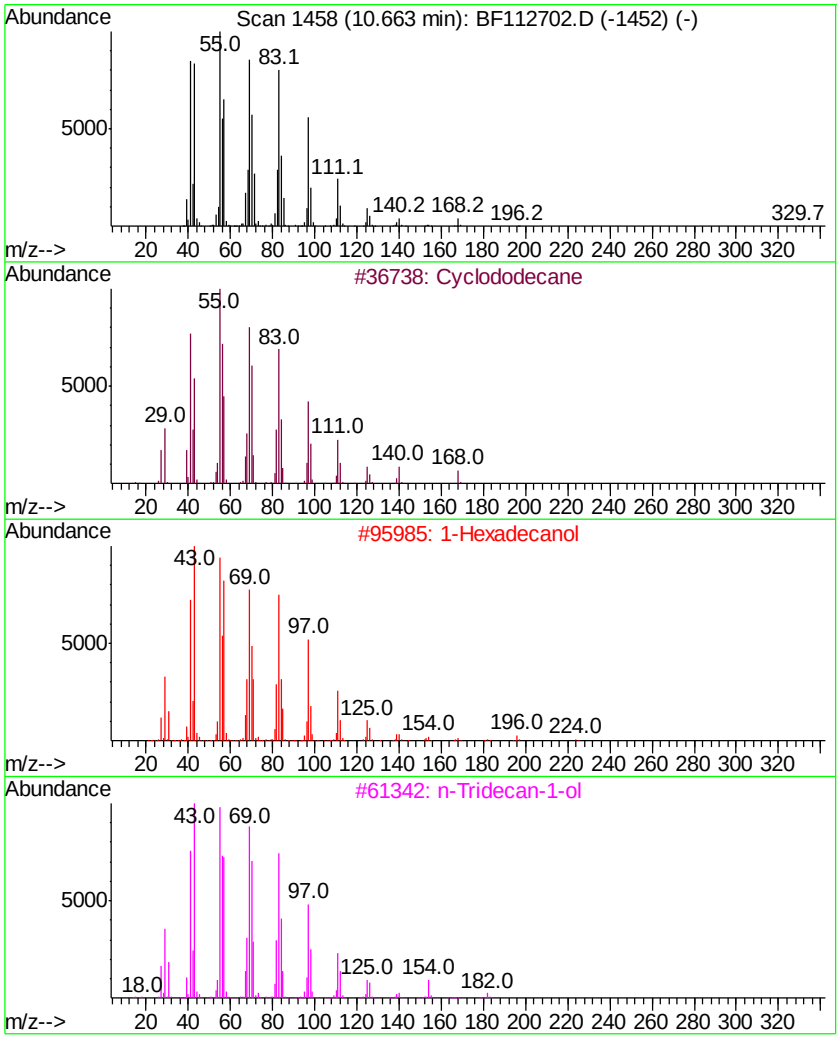
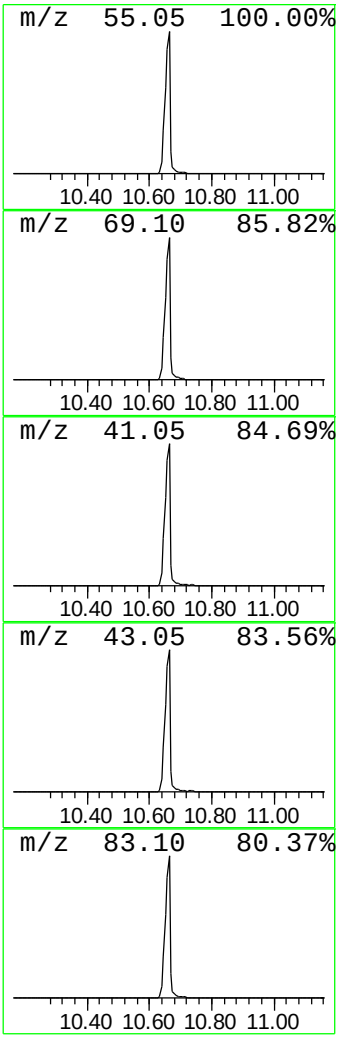
Peak Number 15 Cyclododecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	390.34 ng	7473460	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
4	n-Pentadecanol	228	C15H32O	000629-76-5	91
5	1-Tetradecanol	214	C14H30O	000112-72-1	91





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-022019

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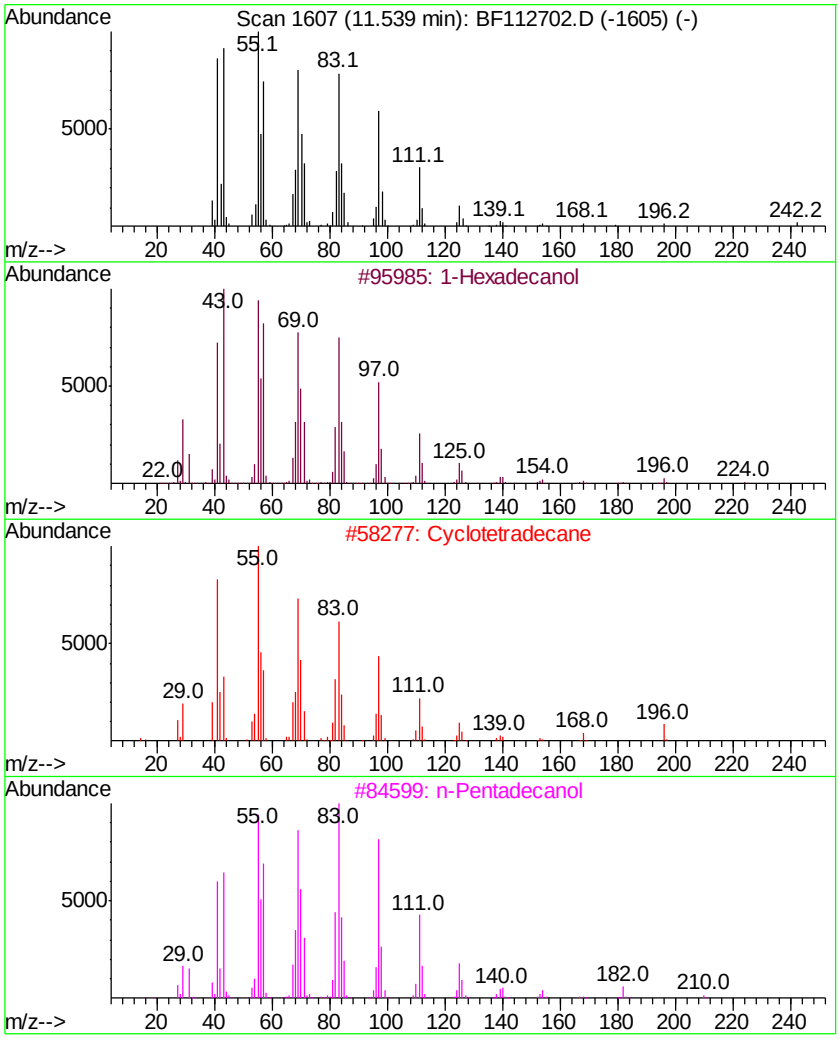
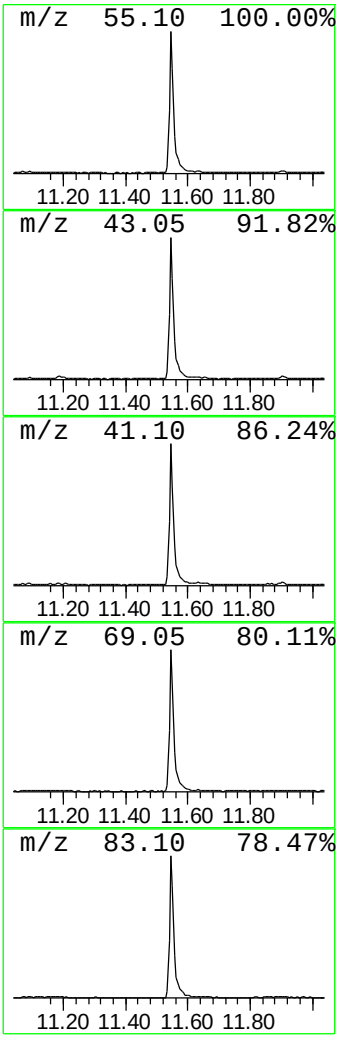
Peak Number 16 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	83.43 ng	1597300	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	Cyclotetradecane	196	C14H28	000295-17-0	95
3	n-Pentadecanol	228	C15H32O	000629-76-5	94
4	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	94
5	1-Tetradecanol	214	C14H30O	000112-72-1	94





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ClientSampleId : NB-022019

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TIC Integration Parameters: LSCINT.P

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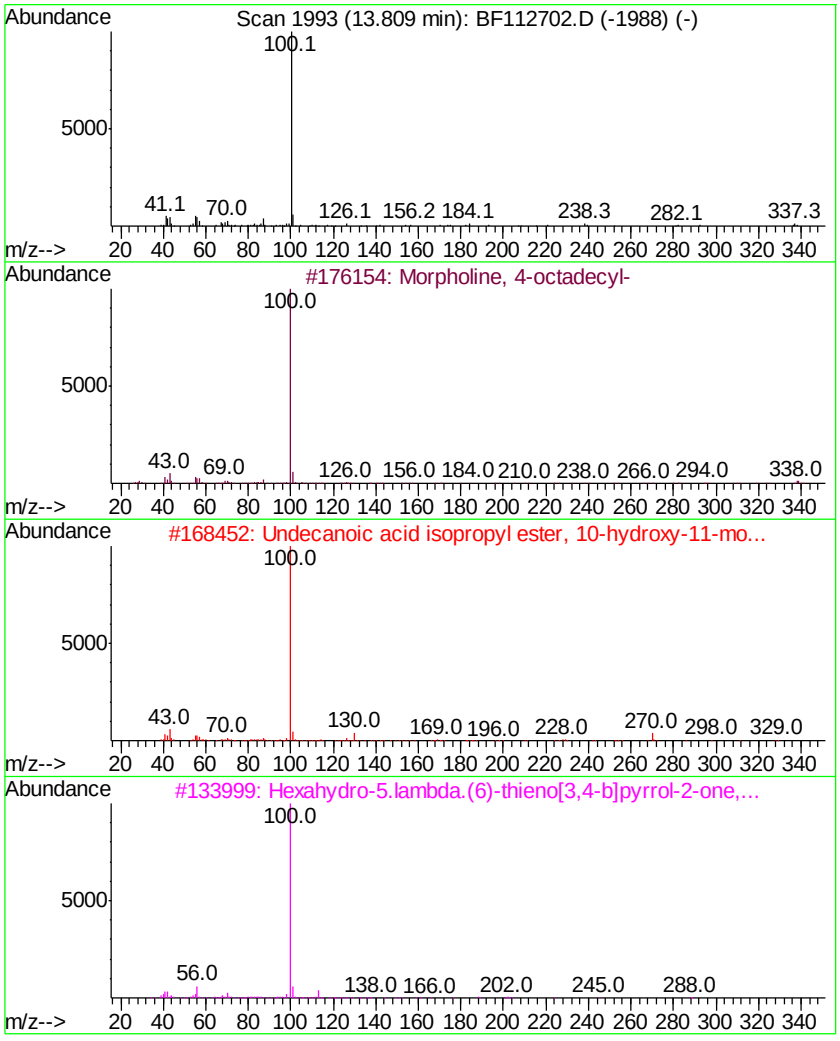
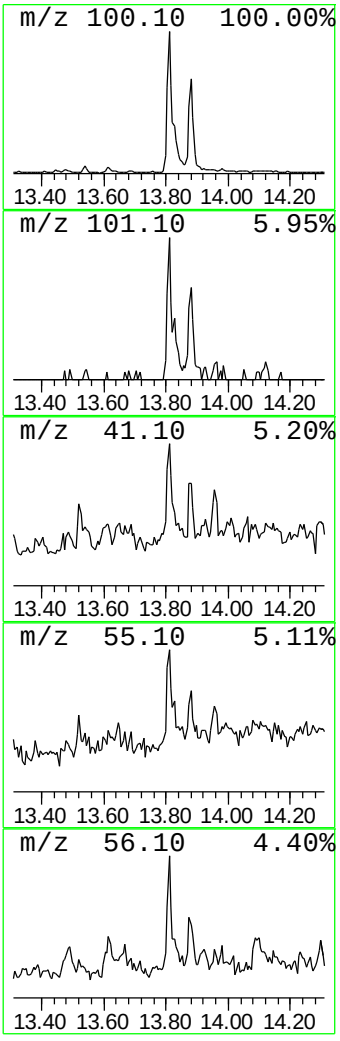
Peak Number 17 Morpholine, 4-octadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	9.05 ng	224779	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-octadecyl-	339	C22H45NO	016528-77-1	64
2	Undecanoic acid isopropyl ester,...	329	C18H35NO4	1000303-32-4	64
3	Hexahydro-5.lambda.(6)-thieno[3,...	288	C12H20N2O4S	1000303-88-9	50
4	Undecanoic acid propyl ester, 10...	329	C18H35NO4	1000303-32-0	50
5	1-Morpholinopropan-2-ol trifluor...	241	C9H14F3NO3	1000373-15-2	50





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TIC Integration Parameters: LSCINT.P

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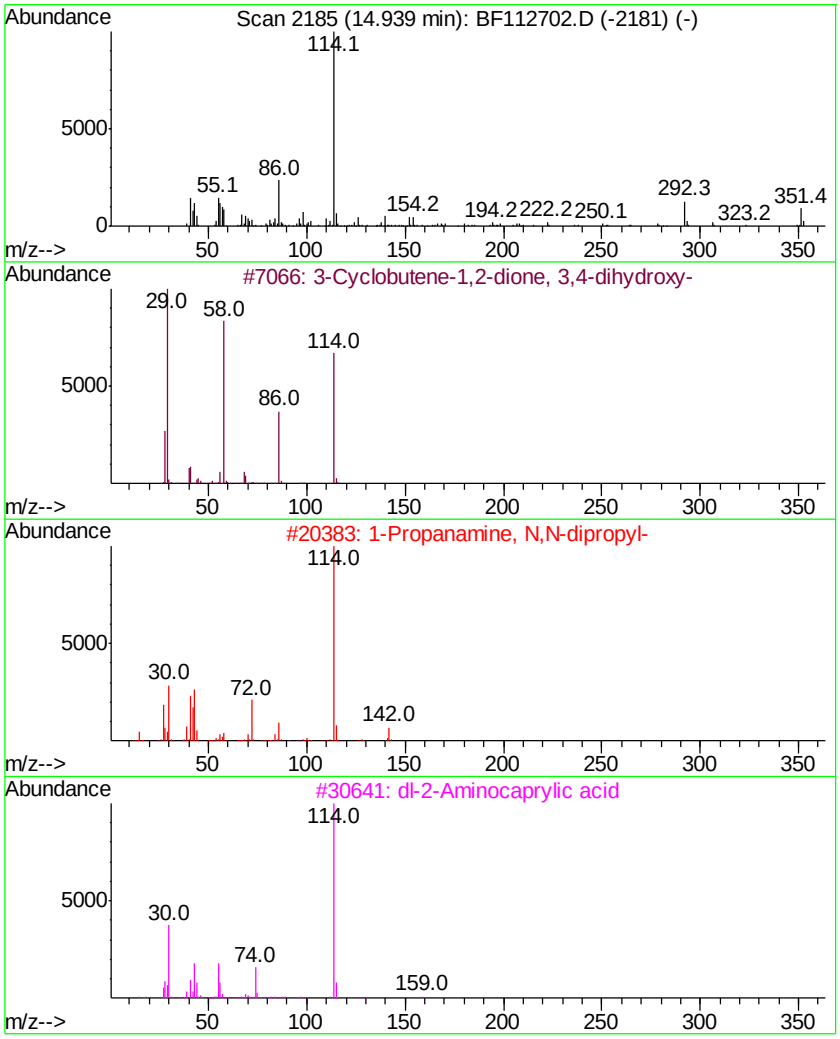
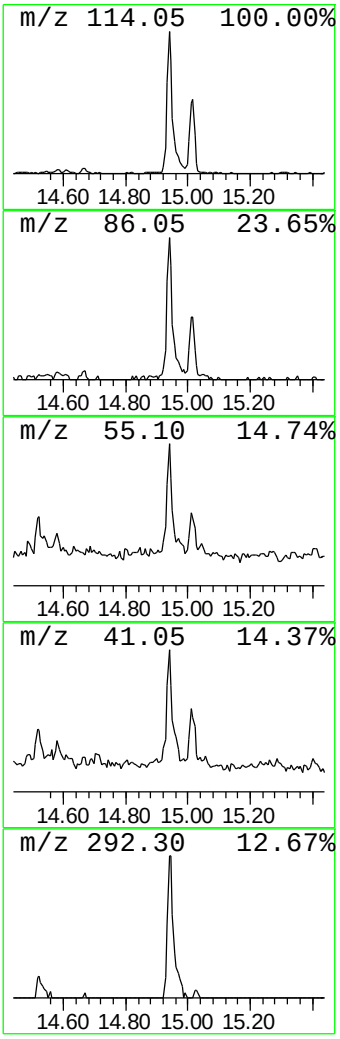
Peak Number 18 3-Cyclobutene-1,2-dione, 3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	17.03 ng	302932	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclobutene-1,2-dione, 3,4-dih...	114	C4H2O4	002892-51-5	59
2	1-Propanamine, N,N-dipropyl-	143	C9H21N	000102-69-2	49
3	dl-2-Aminocaprylic acid	159	C8H17NO2	000644-90-6	47
4	Silacyclooctan-5-one, 1,1-dimethyl-	170	C9H18OSi	010325-31-2	47
5	2H-Imidazole-2-thione, 1,3-dihyd...	114	C4H6N2S	000060-56-0	47





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-Propanol, 1-(2-...	6.62	16.4	ng	286778	1	6.82	348742	20.0
2-Propanol, 1-(2-...	6.74	22.8	ng	397202	1	6.82	348742	20.0
unknown7.73	7.73	2.3	ng	189539	2	8.10	1617130	20.0
unknown7.83	7.83	5.4	ng	435512	2	8.10	1617130	20.0
1,2-Cyclohexanedione	7.90	2.7	ng	217395	2	8.10	1617130	20.0
1-Dodecanol, 3,7,...	7.93	5.0	ng	407840	2	8.10	1617130	20.0
Cyclopentane, 1-e...	7.99	24.6	ng	1985590	2	8.10	1617130	20.0
1-Hexene, 3,3-dim...	8.03	33.0	ng	2670090	2	8.10	1617130	20.0
2-Decene, 7-methy...	8.16	6.5	ng	528449	2	8.10	1617130	20.0
Cyclooctane	8.19	13.7	ng	1107440	2	8.10	1617130	20.0
6-Dodecanol	8.26	11.9	ng	961261	2	8.10	1617130	20.0
1-Decanol	8.52	16.7	ng	1352620	2	8.10	1617130	20.0
Cyclododecane	10.66	390.3	ng	7473460	4	11.34	382916	20.0
1-Hexadecanol	11.54	83.4	ng	1597300	4	11.34	382916	20.0
Morpholine, 4-oct...	13.81	9.1	ng	224779	5	13.99	496494	20.0
3-Cyclobutene-1,2...	14.94	17.0	ng	302932	6	15.46	355751	20.0