LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123968.D
Acq On : 17 May 2021 17:45
Operator : JU/CG
Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CONCESSION-CP-4

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	14	20	rVB	494944	631320	48.35%	6.701%
2	2.281	29	33	37	rVB	38492	46335	3.55%	0.492%
3	5.116	513	515	519	rVB2	15633	18438	1.41%	0.196%
4	5.516	578	583	586	rBV	1117873	966287	74.01%	10.256%
5	6.522	749	754	757	rBV	1064816	1002665	76.79%	10.642%
6	6.722	785	788	794	rBV	47468	38832	2.97%	0.412%
7	6.904	815	819	822	rBV	355671	279265	21.39%	2.964%
8	7.463	909	914	917	rBV	781989	662740	50.76%	7.034%
9	8.186	1033	1037	1040	rBV	453786	354588	27.16%	3.763%
10	9.263	1216	1220	1223	rBV	1563312	1210120	92.68%	12.844%
11	9.651	1283	1286	1289	rBV	182335	125446	9.61%	1.331%
12	9.939	1332	1335	1339	rBV	511477	422958	32.39%	4.489%
13	10.727	1465	1469	1472	rBV	1018735	806631	61.78%	8.561%
14	11.427	1584	1588	1591	rBV	576082	437869	33.54%	4.647%
15	11.951	1674	1677	1682	rBV	71280	63996	4.90%	0.679%
16	13.015	1854	1858	1861	rBV	1610164	1305673	100.00%	13.858%
17	13.910	2006	2010	2019	rBV	154563	174414	13.36%	1.851%
18	14.068	2031	2037	2040	rBV	396989	347951	26.65%	3.693%
19	14.545	2113	2118	2124	rBV4	32036	44318	3.39%	0.470%
20	14.704	2141	2145	2150	rVB2	44538	43280	3.31%	0.459%
21	14.939	2181	2185	2190	rVB3	32595	34552	2.65%	0.367%
22	15.562	2285	2291	2295	rBV	278626	360029	27.57%	3.821%
23	16.103	2379	2383	2389	rBV6	13787	26369	2.02%	0.280%
24	17.415	2602	2606	2612	rVB8	9172	17774	1.36%	0.189%

Sum of corrected areas: 9421850

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Misc :
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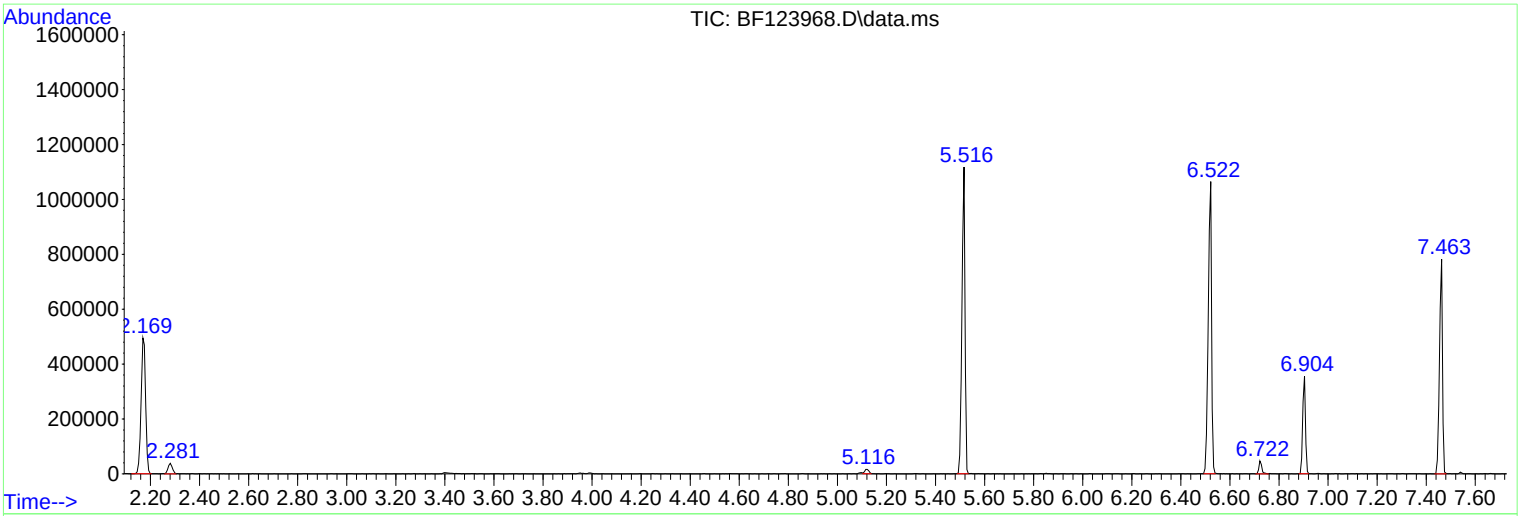
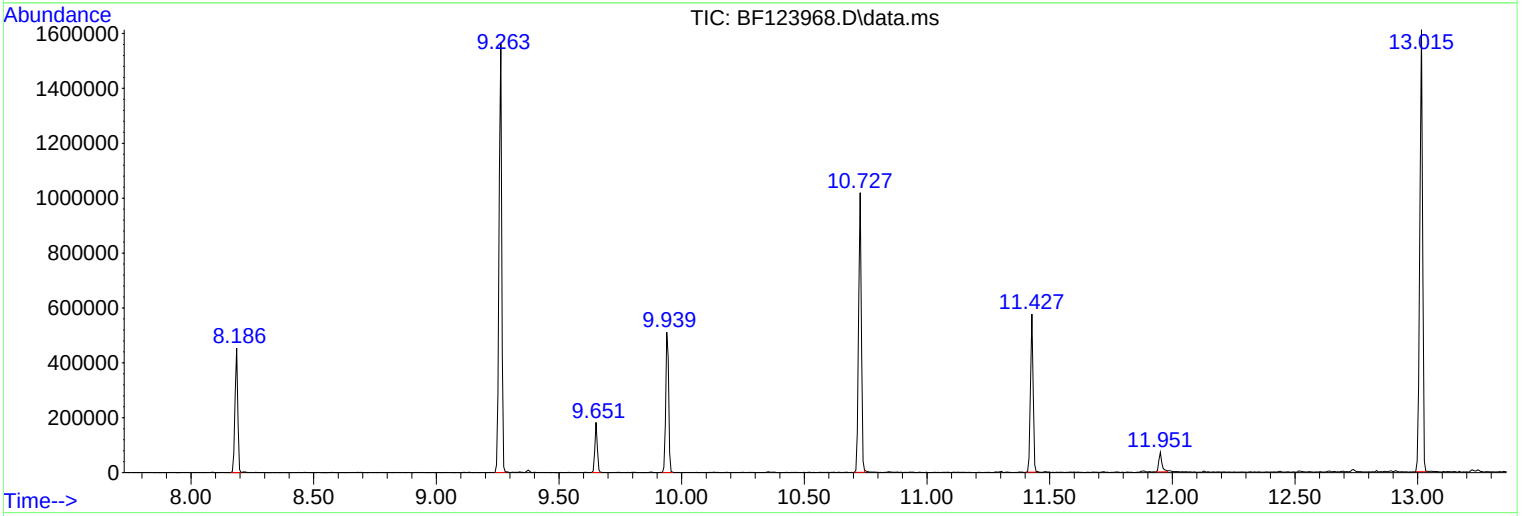
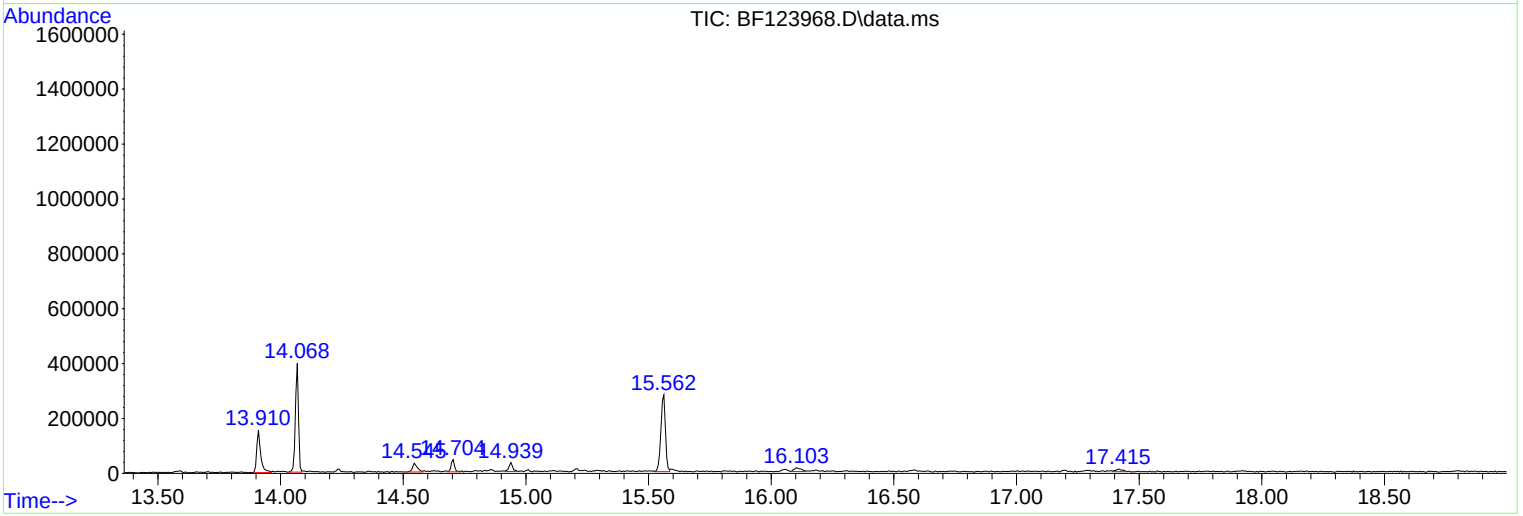
Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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Operator : JU/CG
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Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

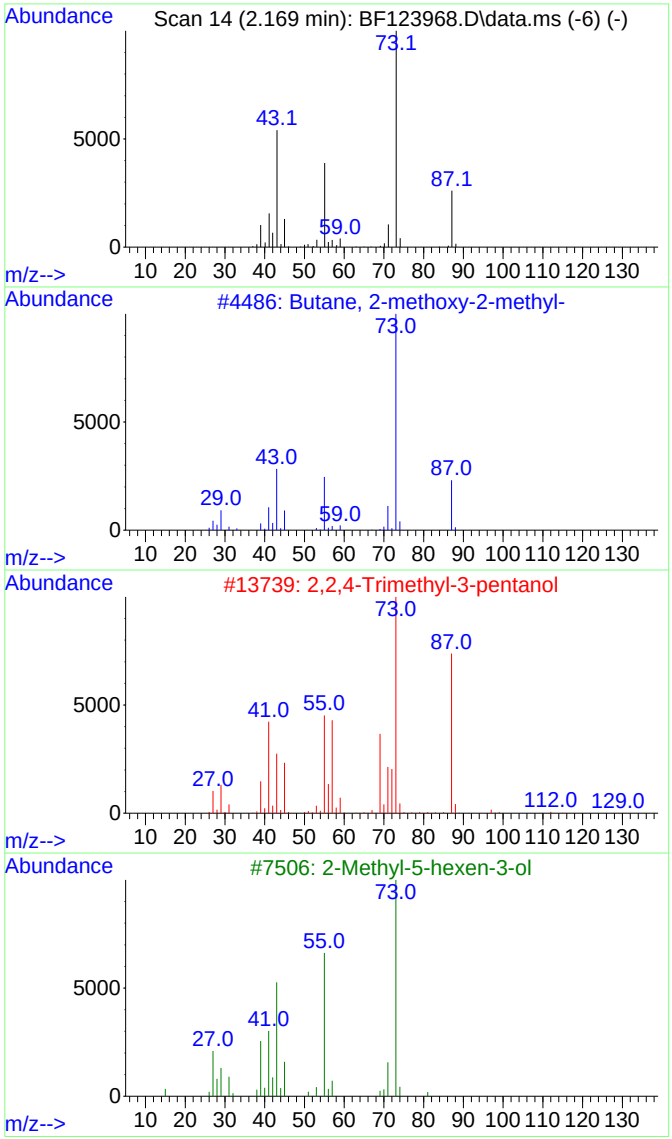
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

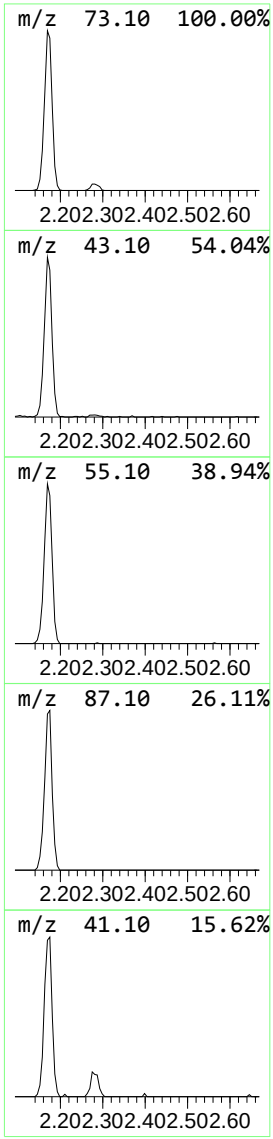
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	45.21 ng	631320	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
4	Propanoic acid, 2-oxo-	88	C3H4O3	000127-17-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF123968.D
Acq On : 17 May 2021 17:45
Operator : JU/CG
Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

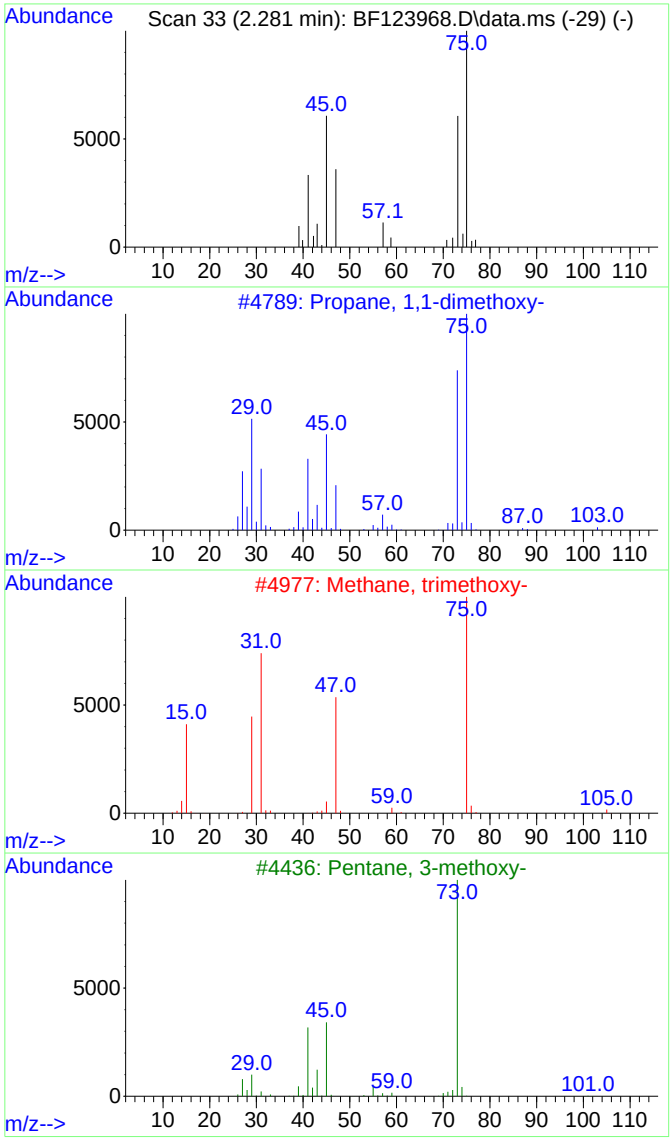
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

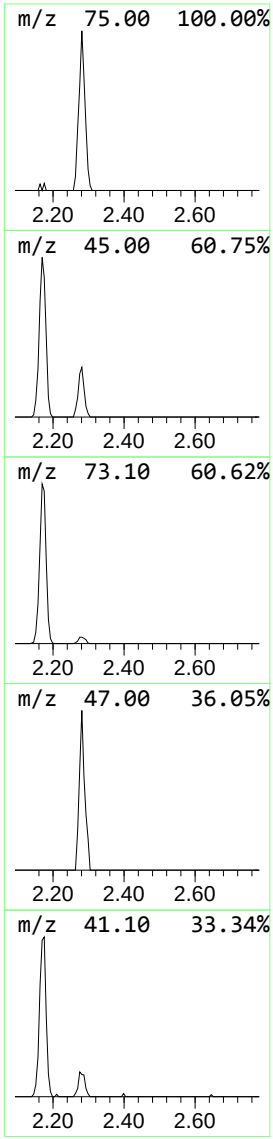
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	3.32 ng	46335	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Methane, trimethoxy-	106	C4H10O3	000149-73-5	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	8
4	Isoxazolidine	73	C3H7NO	000504-72-3	5
5	Formamide, N-methylthio	75	C2H5NS	018952-41-5	5





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Operator : JU/CG
Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

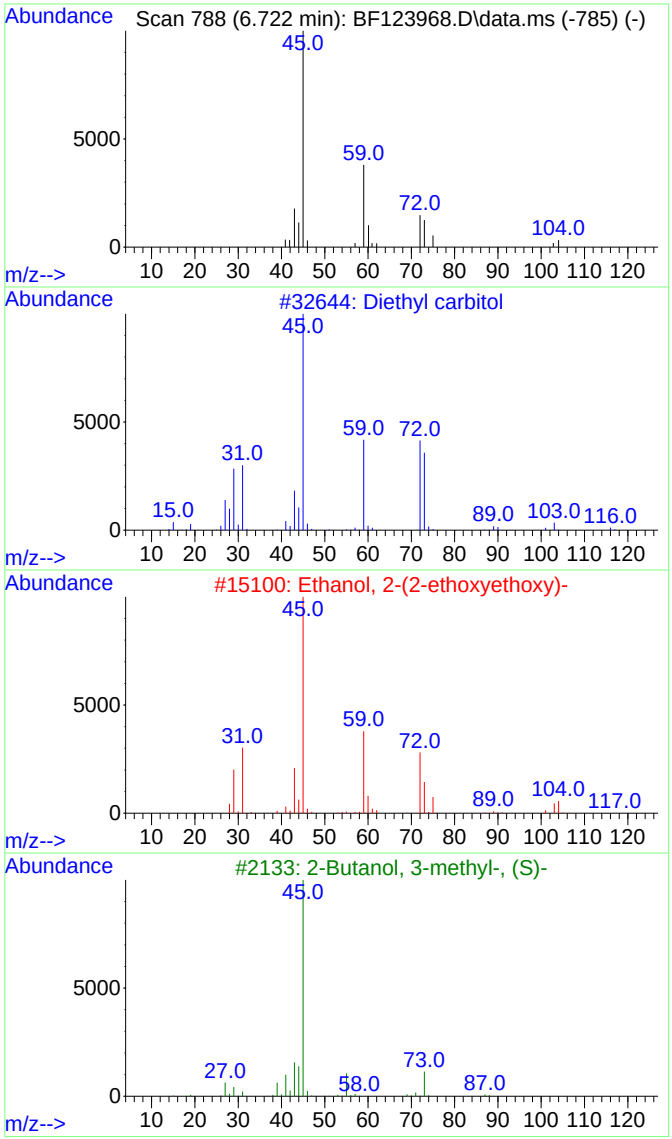
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

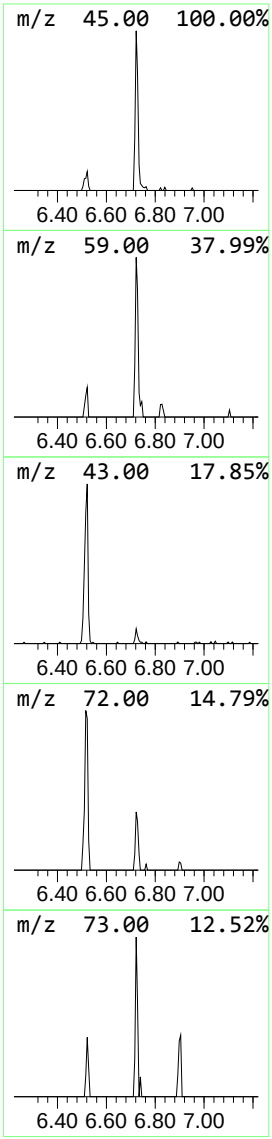
****

Peak Number 3 Diethyl carbitol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	2.78 ng	38832	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl carbitol	162	C8H18O3	000112-36-7	72
2	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	64
3	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	40
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39





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Operator : JU/CG
Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

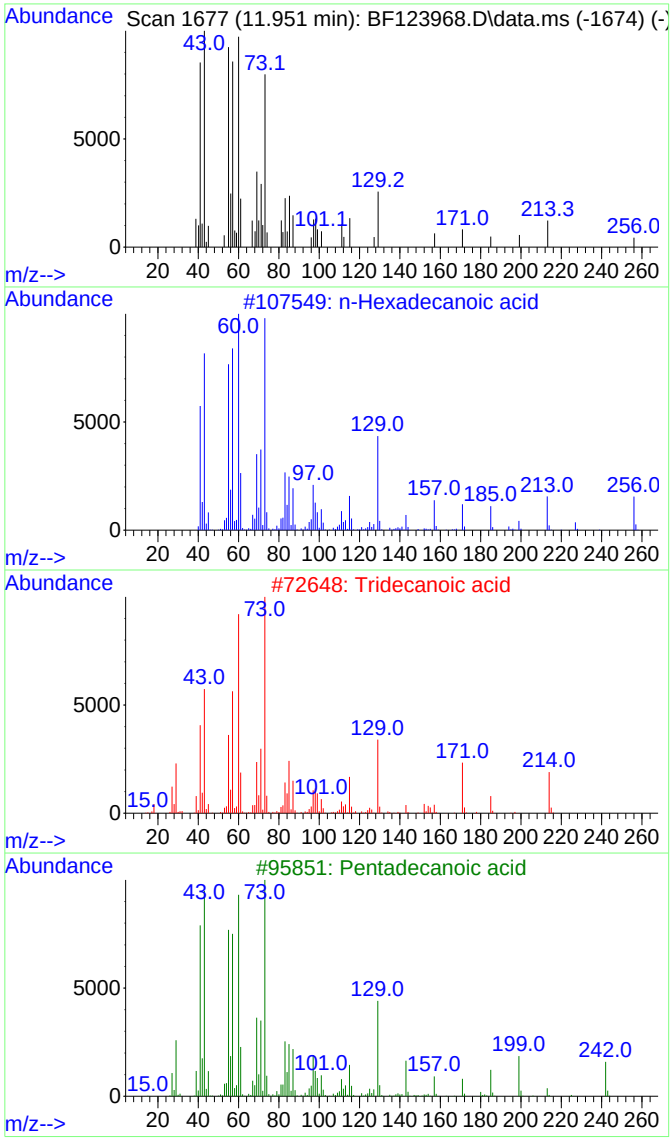
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

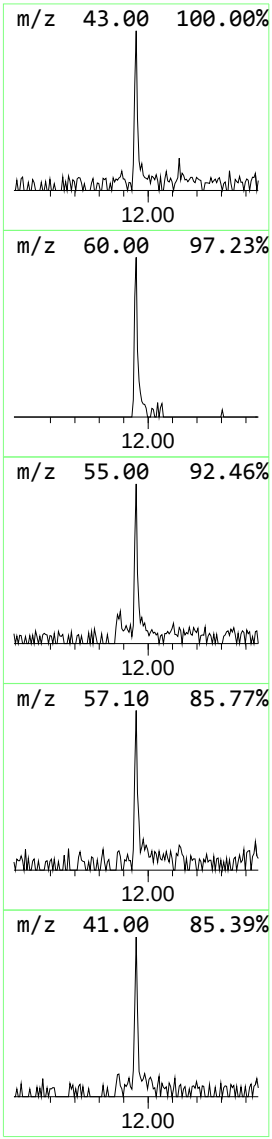
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.92 ng	63996	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Data File : BF123968.D
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Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

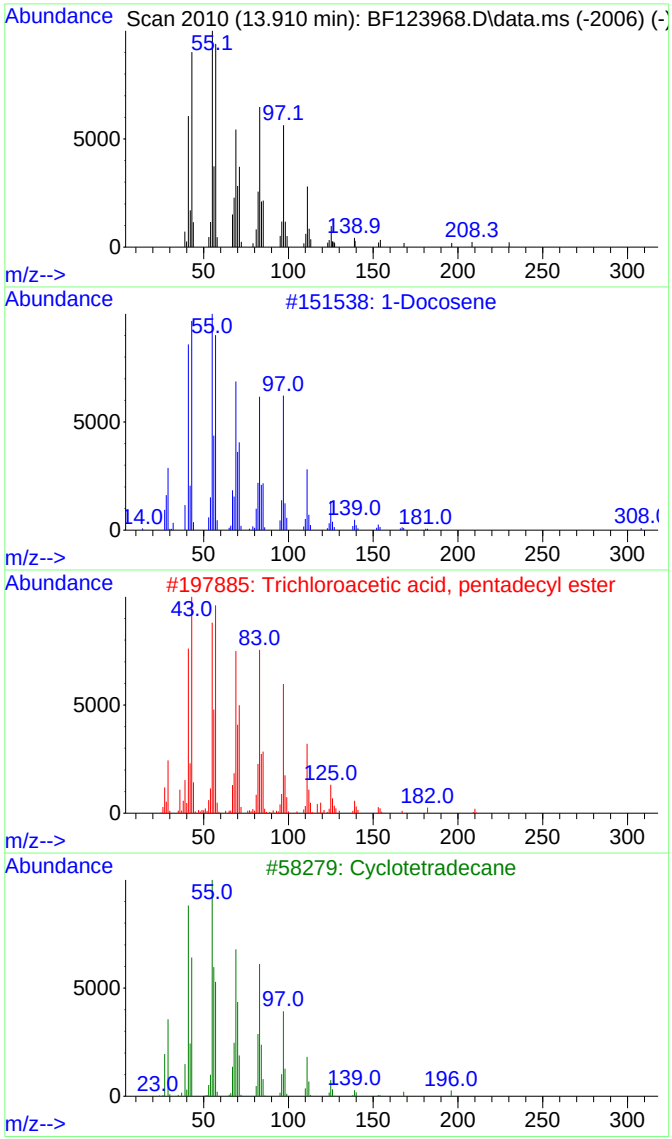
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

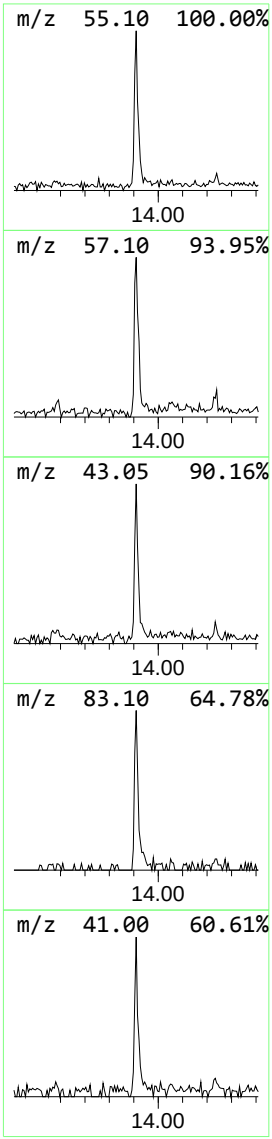
****

Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	10.03 ng	174414	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3	Cyclotetradecane	196	C14H28	000295-17-0	92
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91





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Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

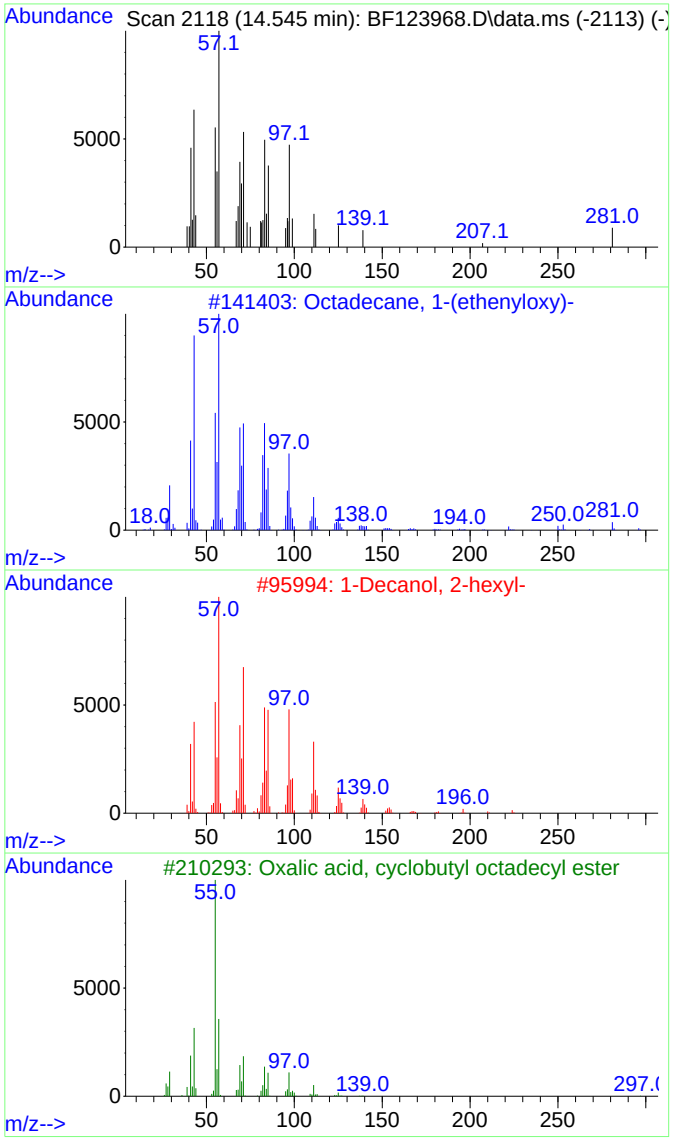
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

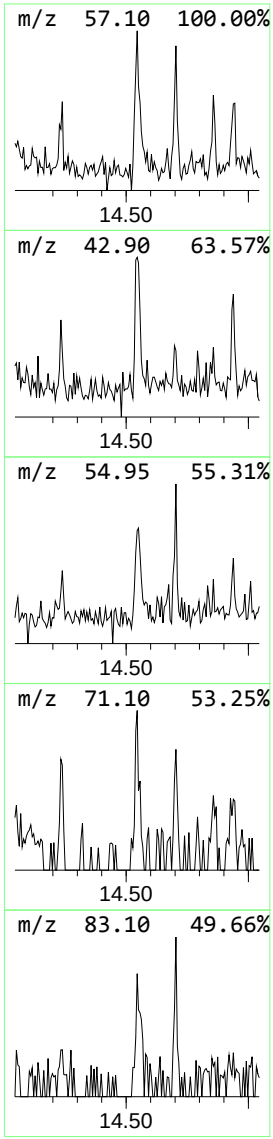
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octadecane, 1-(ethenyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	2.55 ng	44318	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	86
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	80
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	72
4	1-Docosene	308	C22H44	001599-67-3	58
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	58





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Operator : JU/CG
Sample : M2420-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

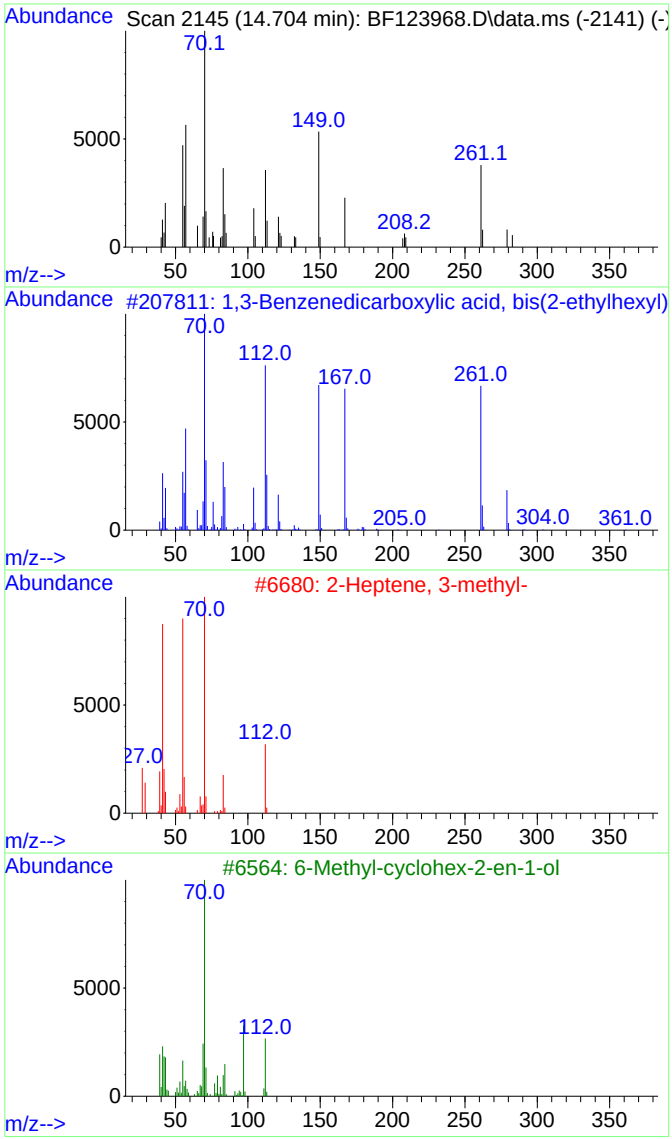
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

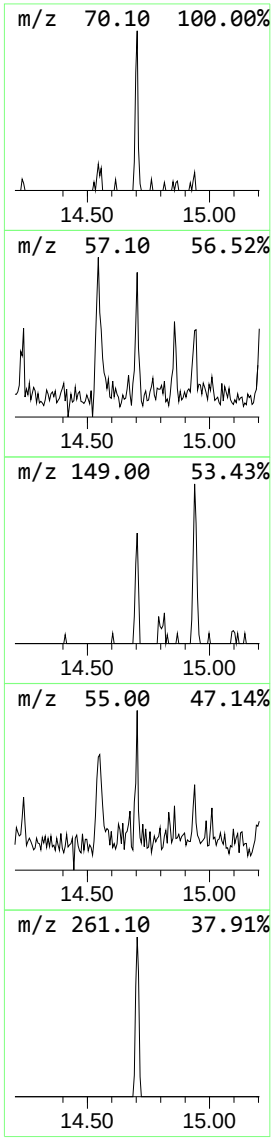
****

Peak Number 7 unknown14.70 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	2.49 ng	43280	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	38
3	6-Methyl-cyclohex-2-en-1-ol	112	C7H12O	1000144-17-3	35
4	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	27
5	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	25





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
Butane, 2-metho...	2.169	45.2	ng	631320	1	6.904	279265	20.0
Propane, 1,1-di...	2.281	3.3	ng	46335	1	6.904	279265	20.0
Diethyl carbitol	6.722	2.8	ng	38832	1	6.904	279265	20.0
n-Hexadecanoic ...	11.951	2.9	ng	63996	4	11.427	437869	20.0
1-Docosene	13.910	10.0	ng	174414	5	14.068	347951	20.0
Octadecane, 1-(...	14.545	2.5	ng	44318	5	14.068	347951	20.0
unknown14.70	14.704	2.5	ng	43280	5	14.068	347951	20.0