LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052621\
Data File : BF124065.D
Acq On : 26 May 2021 15:10
Operator : JU/CG
Sample : M2525-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-5

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: BF124065.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rBV	492869	614034	44.94%	6.022%
2	2.275	27	32	37	rVB	29796	36265	2.65%	0.356%
3	5.110	509	514	521	rVB	393406	458486	33.56%	4.497%
4	5.510	578	582	586	rBV	1129729	1110305	81.27%	10.889%
5	5.904	646	649	653	rBV	42611	37038	2.71%	0.363%
6	6.516	748	753	760	rBV	1072407	1121285	82.07%	10.997%
7	6.722	785	788	793	rBV3	13732	20115	1.47%	0.197%
8	6.892	813	817	820	rBV	404229	310098	22.70%	3.041%
9	7.451	907	912	915	rBV	871614	769902	56.35%	7.551%
10	8.175	1031	1035	1040	rBV	471797	377409	27.62%	3.701%
11	9.251	1214	1218	1221	rBV	1729301	1366248	100.00%	13.399%
12	9.639	1281	1284	1292	rVB	156728	127813	9.36%	1.254%
13	9.927	1330	1333	1340	rBV	489364	454291	33.25%	4.455%
14	10.722	1463	1468	1478	rBV	963787	917466	67.15%	8.998%
15	11.421	1583	1587	1590	rBV	472344	434042	31.77%	4.257%
16	11.939	1672	1675	1680	rBV	26449	25900	1.90%	0.254%
17	12.633	1790	1793	1797	rBV	17440	16814	1.23%	0.165%
18	12.674	1797	1800	1803	rVV	79906	61766	4.52%	0.606%
19	13.004	1852	1856	1860	rBV	1201795	1140179	83.45%	11.182%
20	13.951	2011	2017	2029	rBV5	47731	149252	10.92%	1.464%
21	14.062	2030	2036	2039	rBV	349646	297955	21.81%	2.922%
22	15.556	2285	2290	2295	rBV2	240135	328491	24.04%	3.222%
23	16.033	2369	2371	2376	rVB6	16378	21134	1.55%	0.207%

Sum of corrected areas: 10196288

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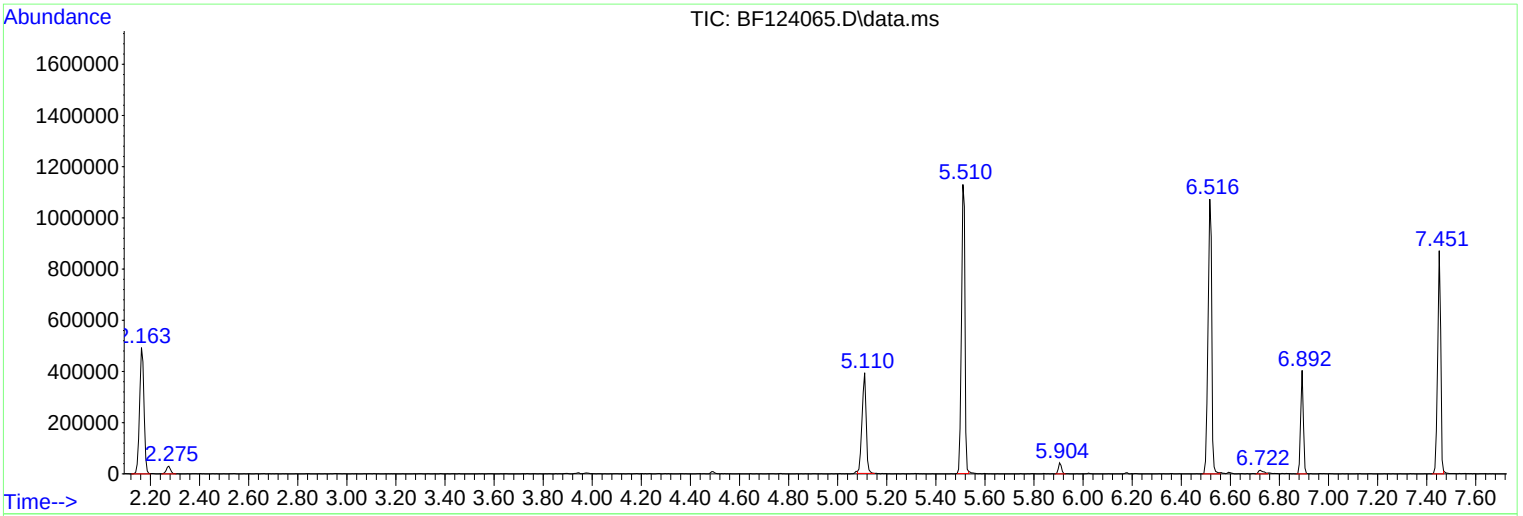
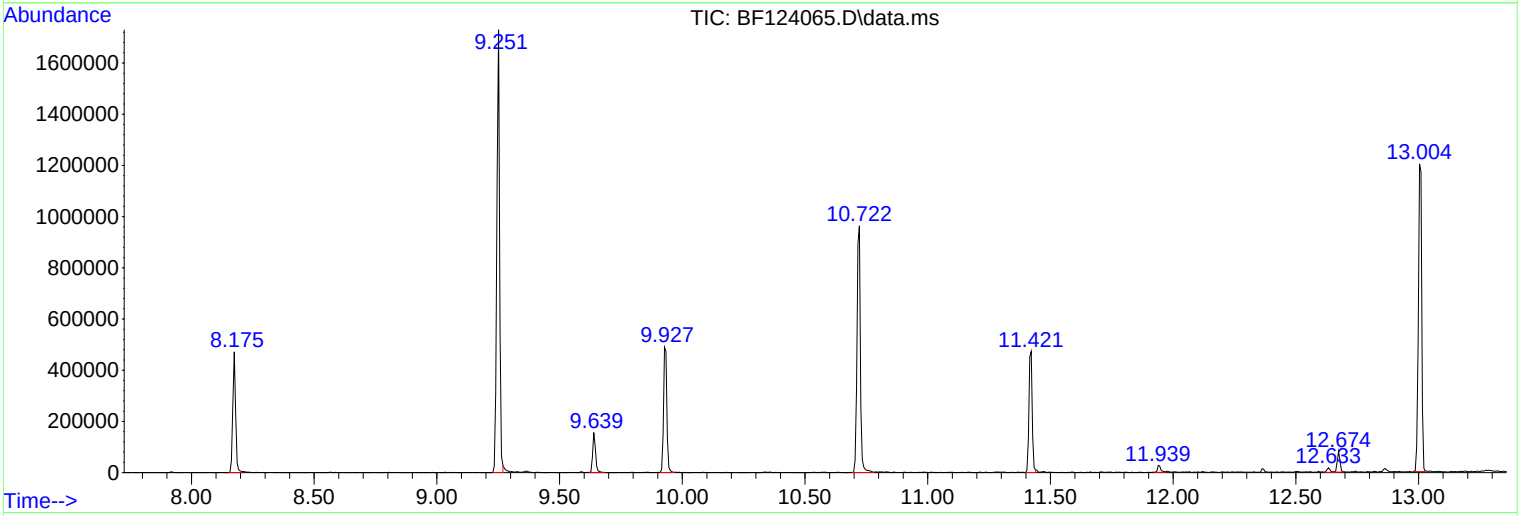
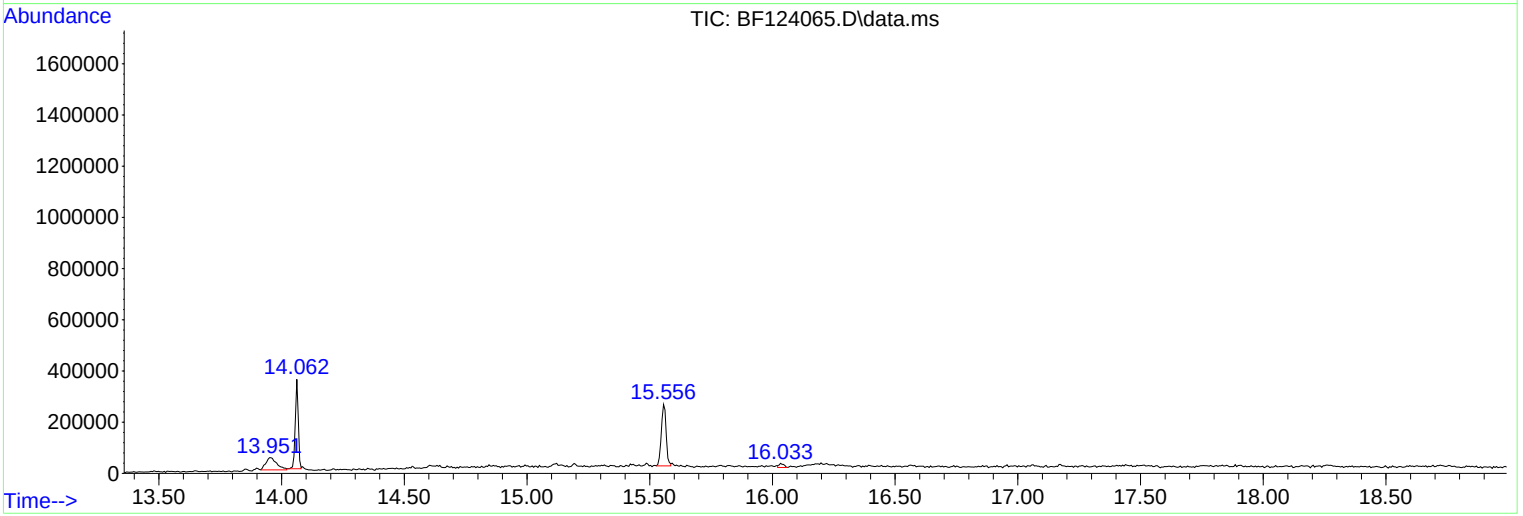
Instrument :
BNA_F
ClientSampleId :
TS-5

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
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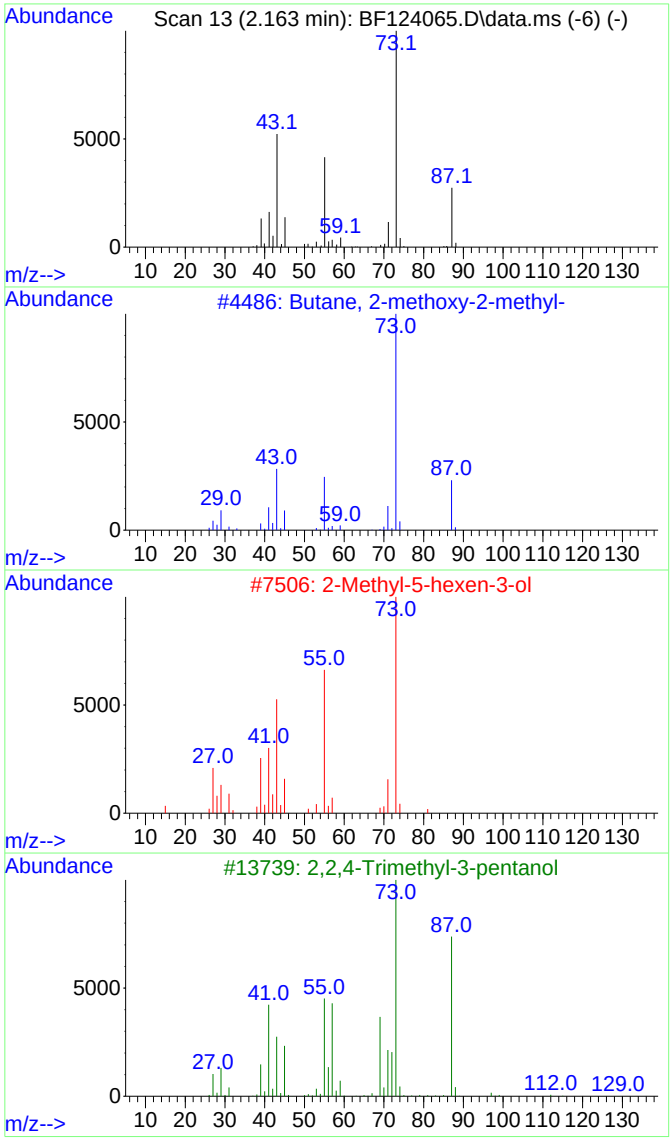
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

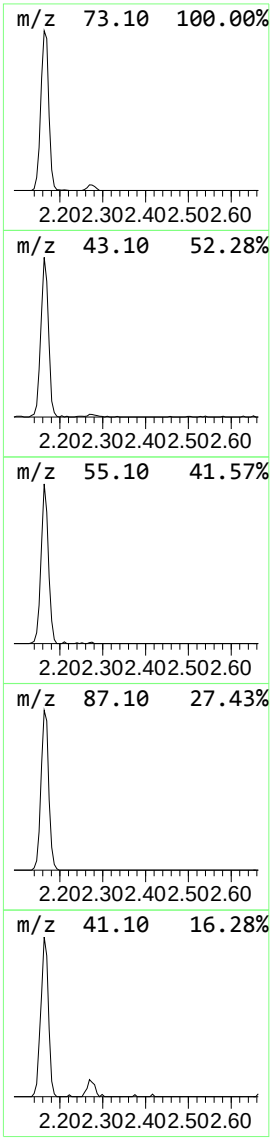
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	39.60 ng	614034	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	Oxirane, [(hexyloxy)methyl]-	158	C9H18O2	005926-90-9	12
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Operator : JU/CG
Sample : M2525-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-5

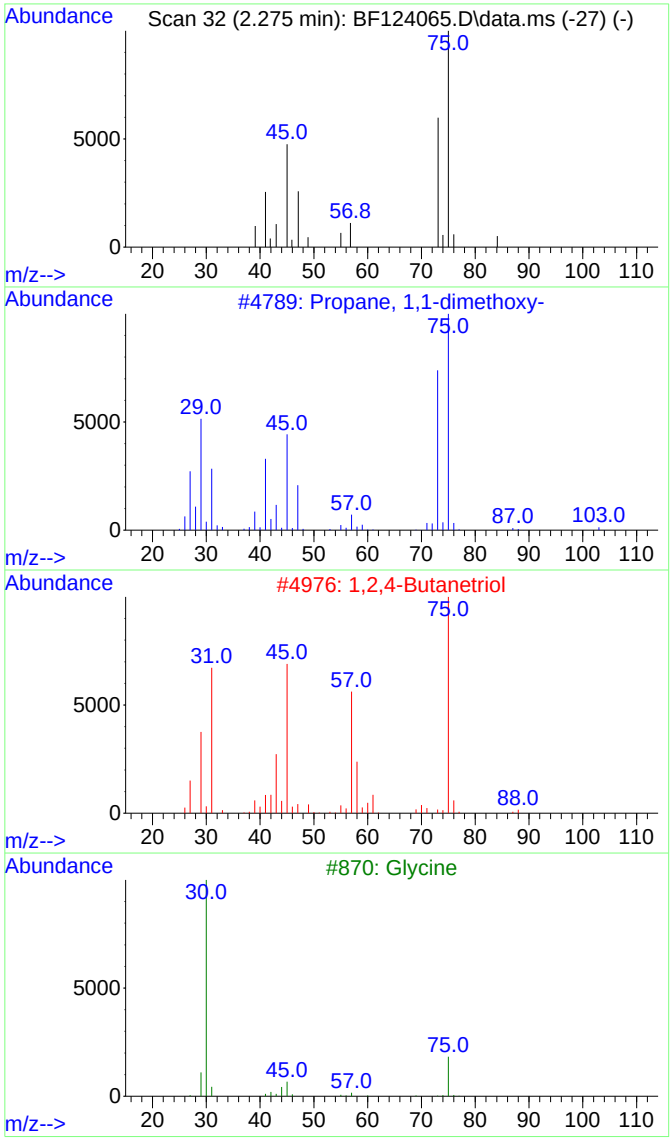
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

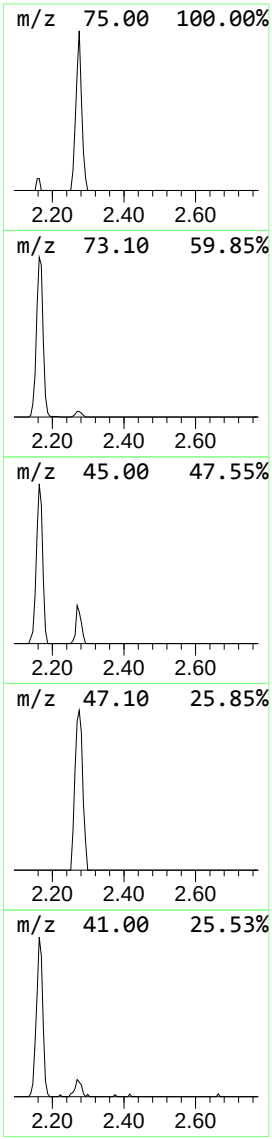
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	2.34 ng	36265	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	1,2,4-Butanetriol	106	C4H10O3	003068-00-6	38
3	Glycine	75	C2H5NO2	000056-40-6	9
4	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9





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Data File : BF124065.D
Acq On : 26 May 2021 15:10
Operator : JU/CG
Sample : M2525-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-5

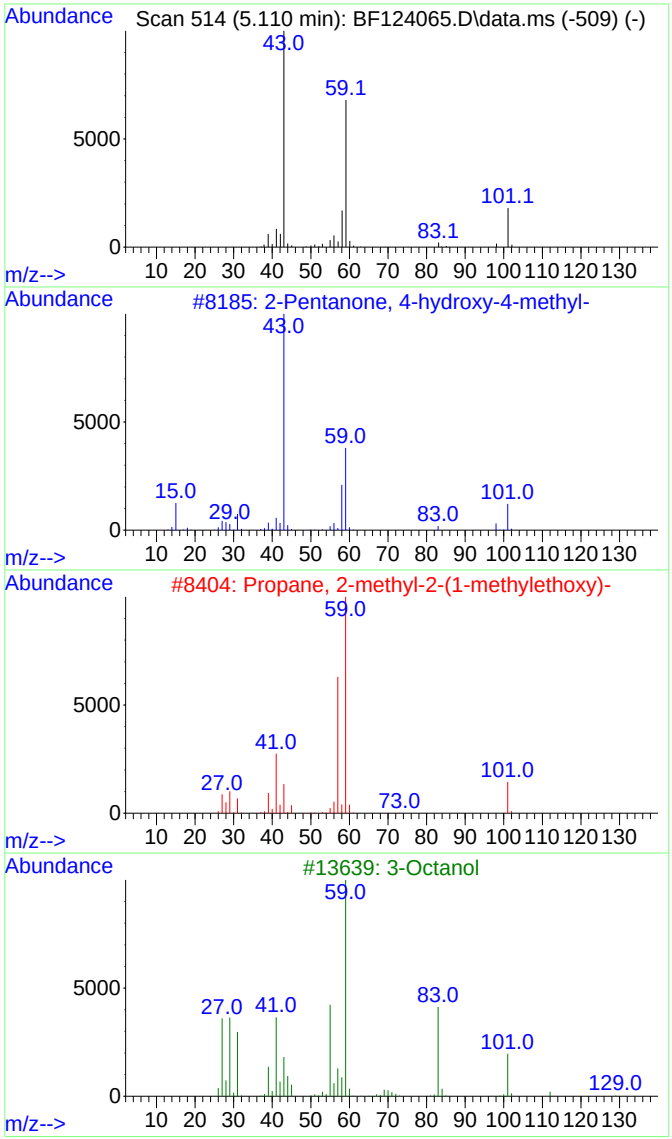
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

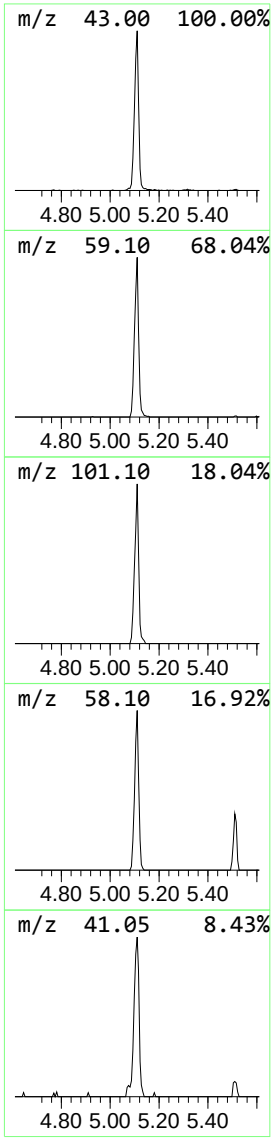
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	29.57 ng	458486	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Sample : M2525-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-5

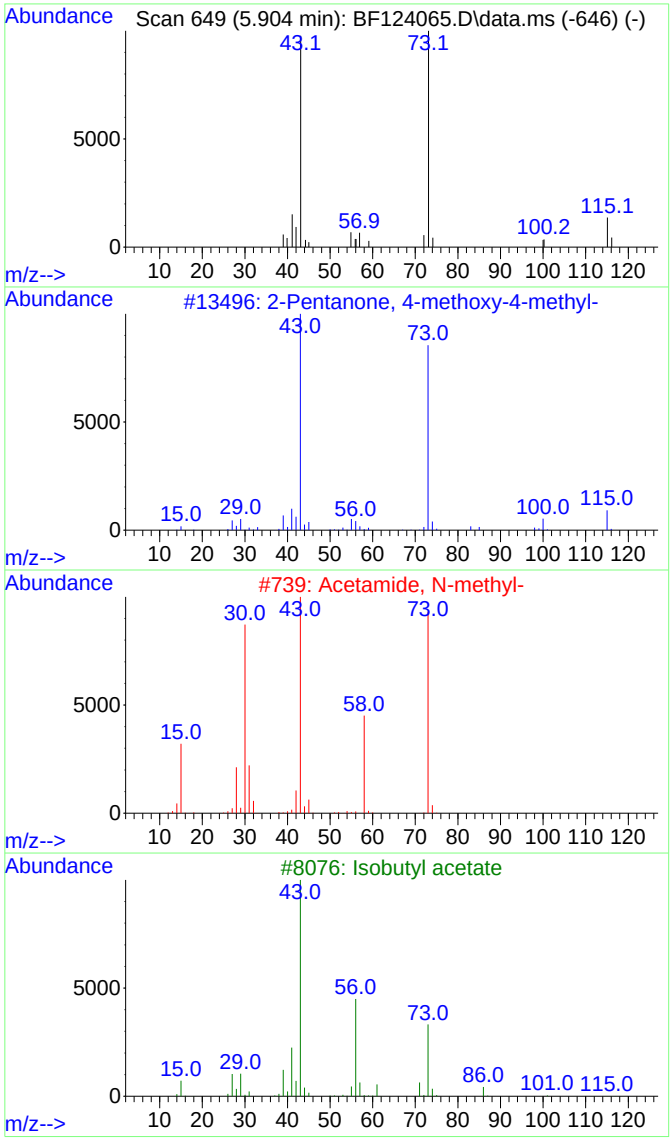
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

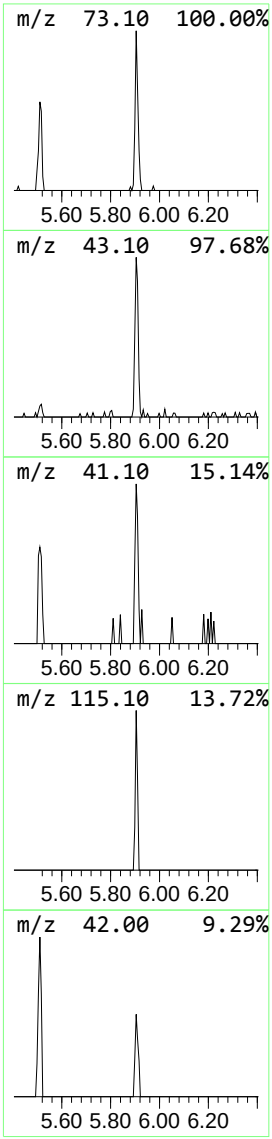
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.904	2.39 ng	37038	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3	Isobutyl acetate	116	C6H12O2	000110-19-0	33
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-5

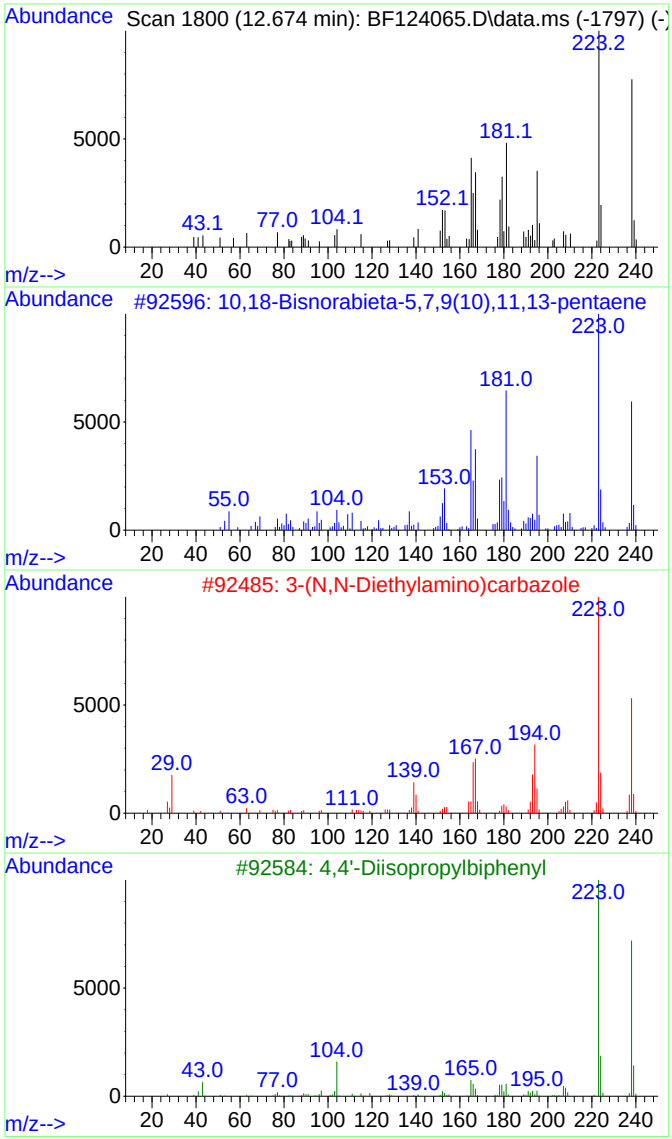
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

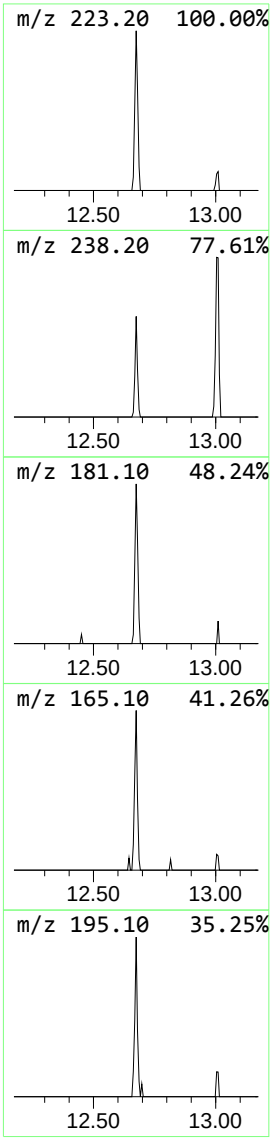
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.85 ng	61766	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	95
2	3-(N,N-Diethylamino)carbazole	238	C16H18N2	054994-31-9	53
3	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	46
4	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	46
5	Ethane, 1-(2,3-xylyl)-1-(3,4-xyl...	238	C18H22	002816-98-0	38





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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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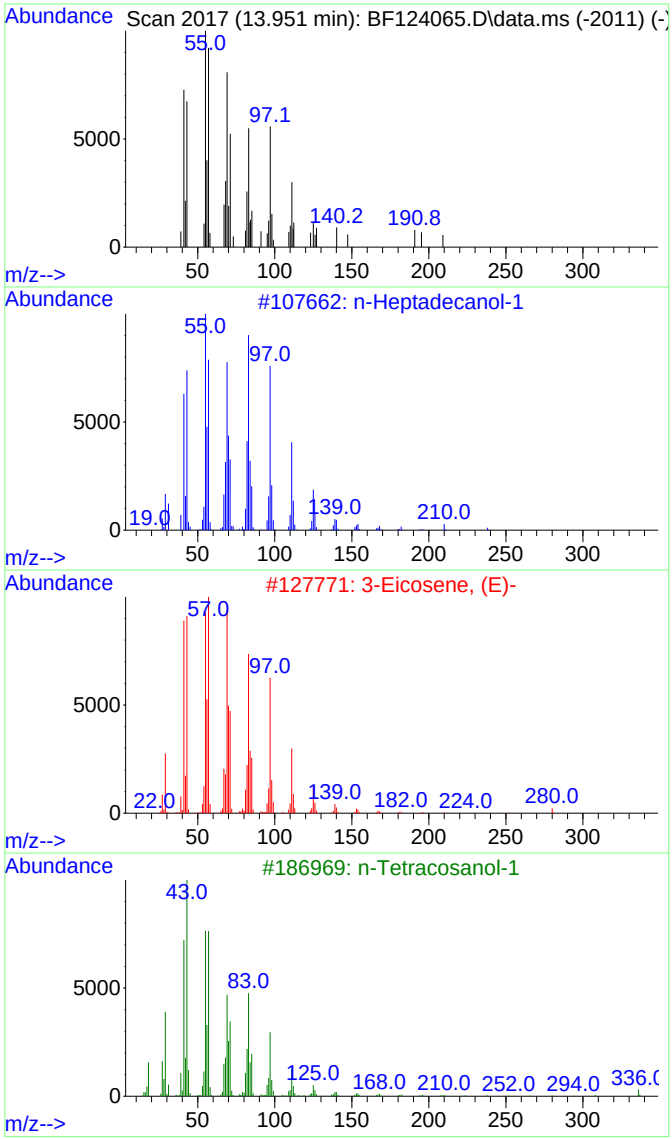
TIC Integration Parameters: LSCINT.P

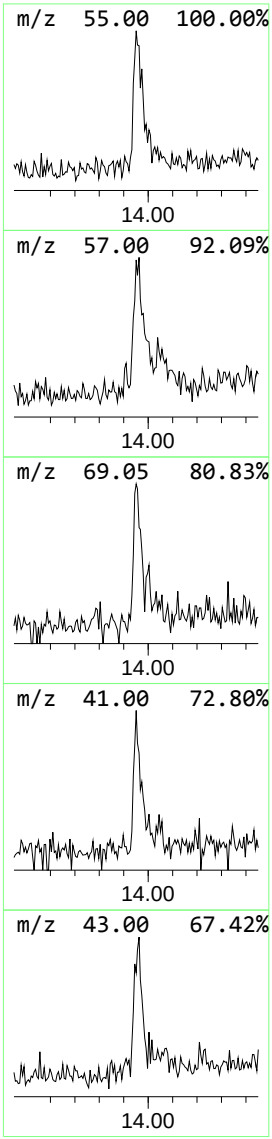
****

Peak Number 6 n-Heptadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	10.02 ng	149252	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	80
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	80
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	74
4	1-Hexadecanol	242	C16H34O	036653-82-4	72
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	58





Tentatively Identified Compound (LSC) summary

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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...	2.163	39.6	ng	614034	1	6.892	310098	20.0
Propane, 1,1-di...	2.275	2.3	ng	36265	1	6.892	310098	20.0
2-Pentanone, 4-...	5.110	29.6	ng	458486	1	6.892	310098	20.0
2-Pentanone, 4-...	5.904	2.4	ng	37038	1	6.892	310098	20.0
10,18-Bisnorabi...	12.674	2.9	ng	61766	4	11.422	434042	20.0
n-Heptadecanol-1	13.951	10.0	ng	149252	5	14.063	297955	20.0