LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082730.D
Acq On : 5 Nov 2015 15:36
Operator : UM/IZ
Sample : G4261-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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-BF103015.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	2.133	3	4	18	rVB2	141121	309766	5.28%	0.602%
2	3.836	149	153	156	rVB	366882	536883	9.15%	1.043%
3	5.059	256	260	270	rVB	1631046	2703659	46.06%	5.253%
4	5.470	293	296	299	rBV	3875507	5219849	88.93%	10.142%
5	6.499	383	386	389	rBV	4395525	4974999	84.75%	9.667%
6	6.636	395	398	400	rBV	5556690	5466951	93.14%	10.623%
7	6.864	416	418	420	rBV	1278882	1024134	17.45%	1.990%
8	6.933	422	424	426	rBV	150289	119407	2.03%	0.232%
9	7.024	429	432	434	rBV	4820011	4240541	72.24%	8.240%
10	7.424	464	467	470	rBV	2870571	3418451	58.24%	6.642%
11	8.156	528	531	533	rBV	972124	1220749	20.80%	2.372%
12	9.230	622	625	628	rBV	6037632	5869881	100.00%	11.406%
13	9.505	647	649	651	rBV	446052	359159	6.12%	0.698%
14	9.619	657	659	662	rBV	1307113	1192724	20.32%	2.318%
15	9.905	682	684	687	rBV	1614964	1406823	23.97%	2.734%
16	10.328	718	721	722	rBV2	117842	131841	2.25%	0.256%
17	10.693	750	753	755	rBV	4079450	4024958	68.57%	7.821%
18	11.391	811	814	815	rBV	1198027	1354898	23.08%	2.633%
19	11.928	859	861	863	rBV2	211071	274524	4.68%	0.533%
20	12.591	917	919	921	rBV	136505	154279	2.63%	0.300%
21	12.705	927	929	931	rBV	79830	94315	1.61%	0.183%
22	12.819	936	939	942	rVV	122372	159498	2.72%	0.310%
23	12.979	950	953	955	rBV	5099015	4983806	84.90%	9.684%
24	13.882	1029	1032	1035	rBV2	82270	150371	2.56%	0.292%
25	14.019	1042	1044	1049	rBV	1056035	1083250	18.45%	2.105%
26	15.460	1167	1170	1173	rVB	718947	989561	16.86%	1.923%

Sum of corrected areas: 51465277

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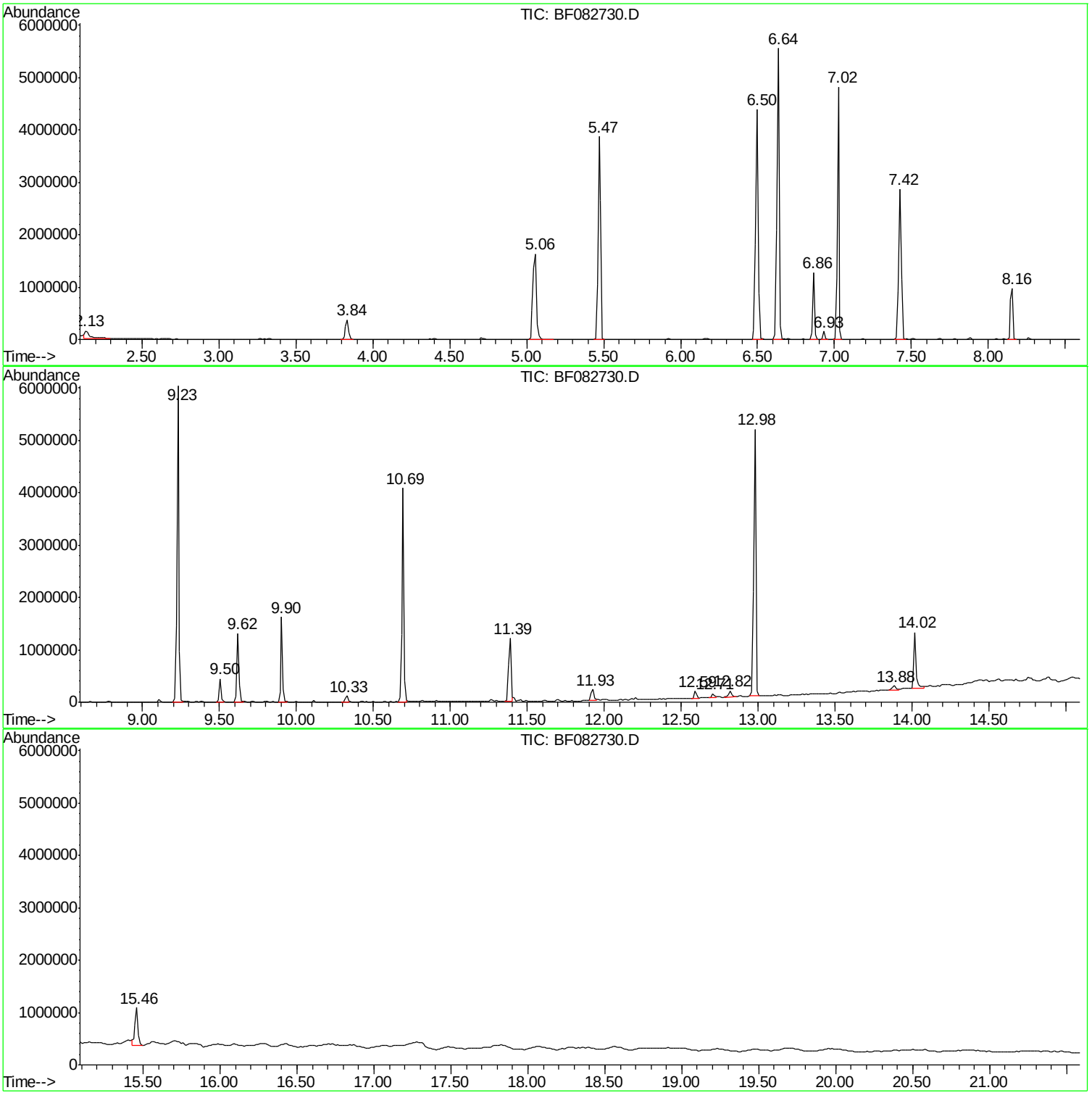
Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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

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Data File : BF082730.D
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Operator : UM/IZ
Sample : G4261-04
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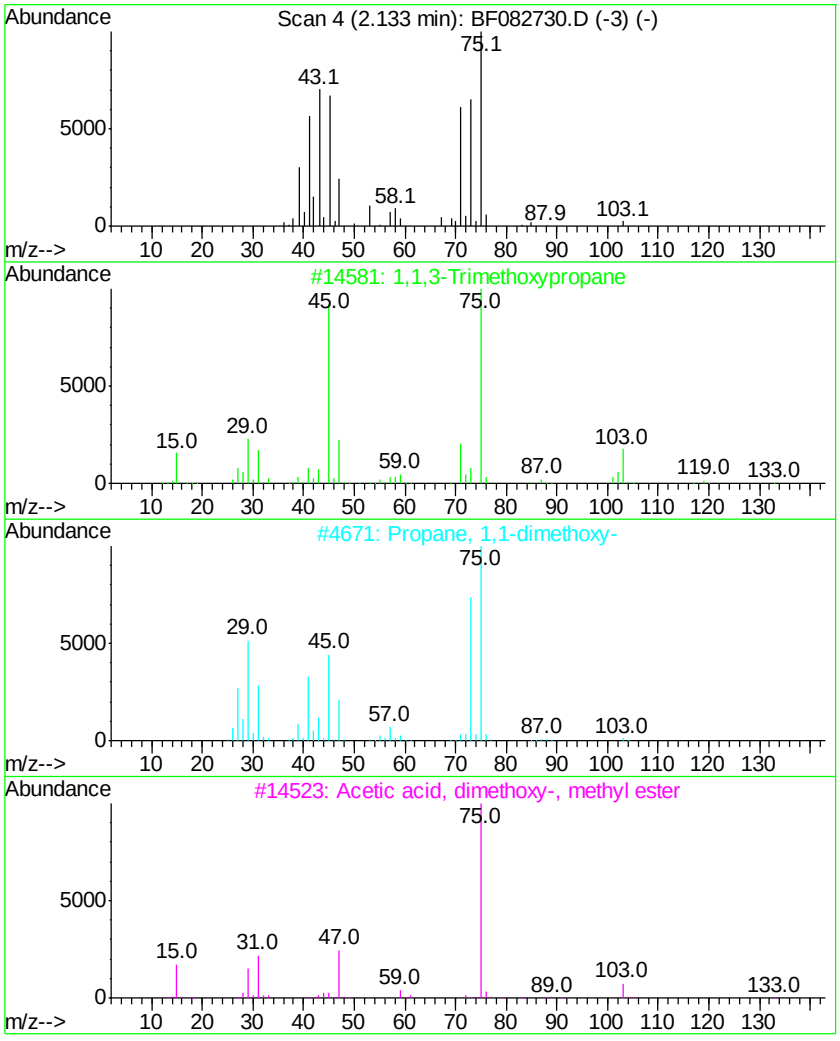
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

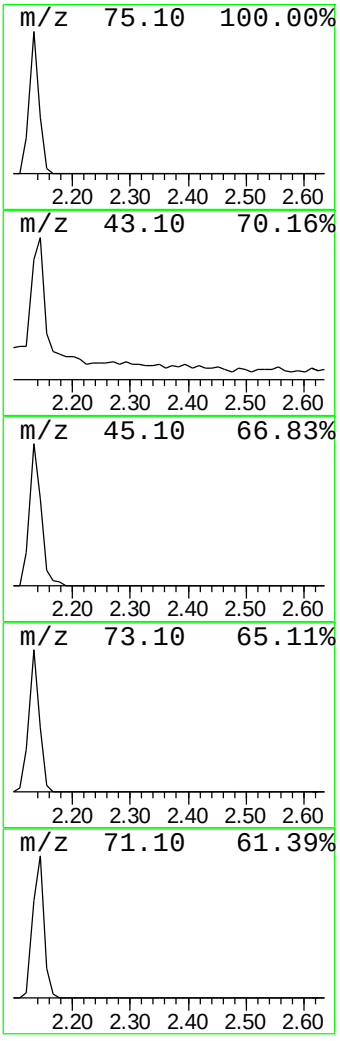
****

Peak Number 1 1,1,3-Trimethoxypropane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	6.05 ng	309766	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,3-Trimethoxypropane	134	C6H14O3	014315-97-0	59
2	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	33
3	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	32
4	1,4-Pentanediol	104	C5H12O2	000626-95-9	16
5	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	12





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Acq On : 5 Nov 2015 15:36
Operator : UM/IZ
Sample : G4261-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

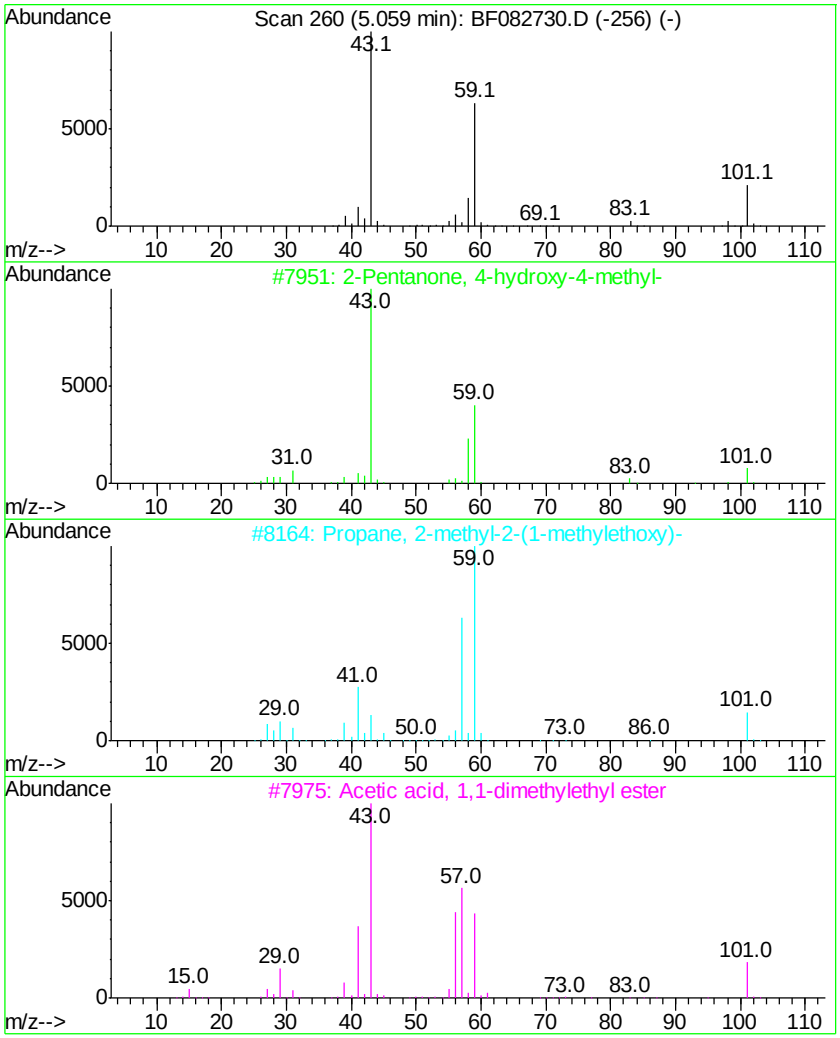
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

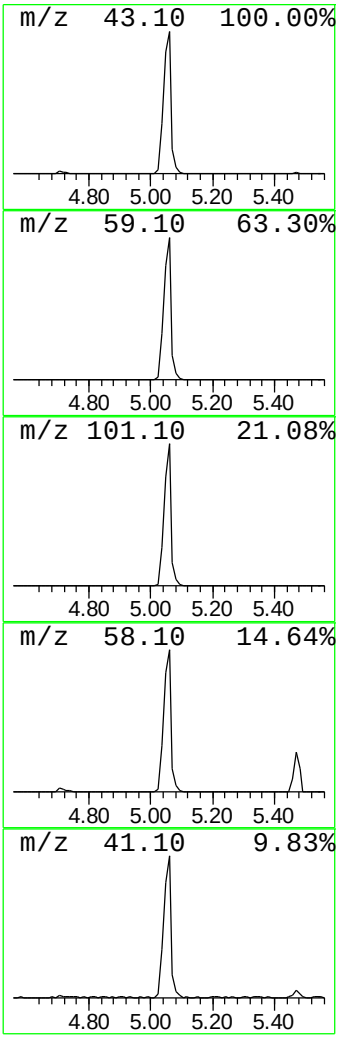
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	52.80 ng	2703660	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082730.D
Acq On : 5 Nov 2015 15:36
Operator : UM/IZ
Sample : G4261-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
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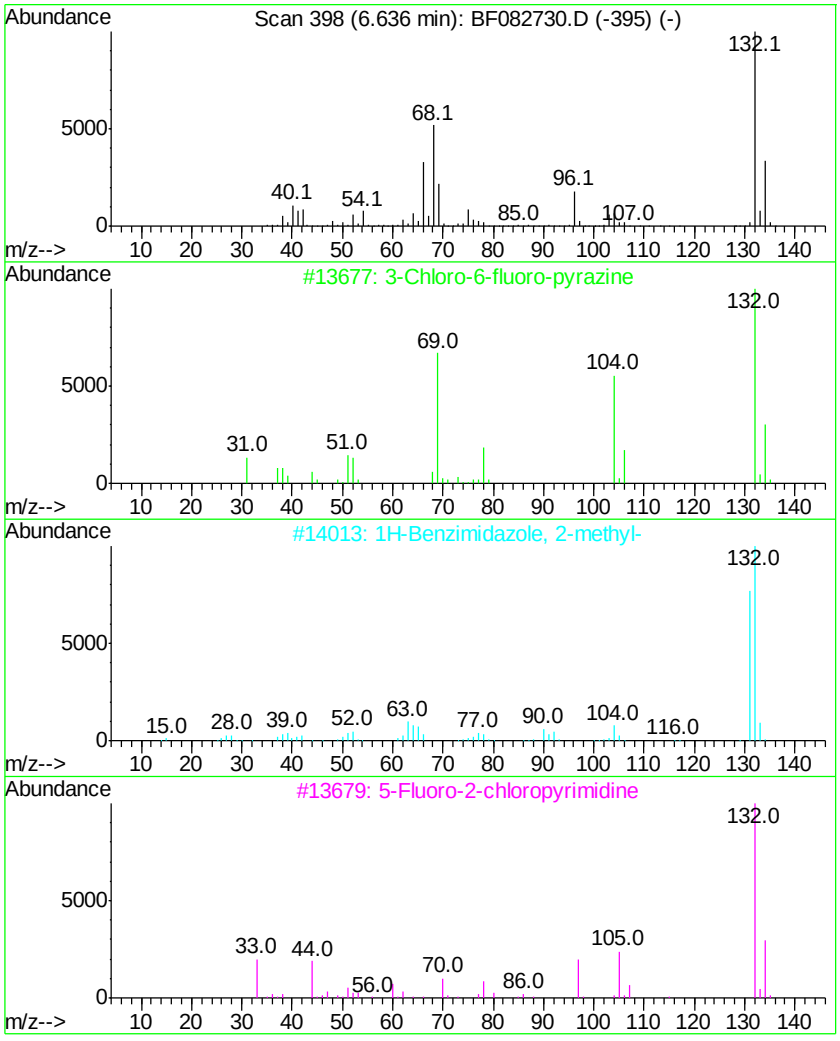
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

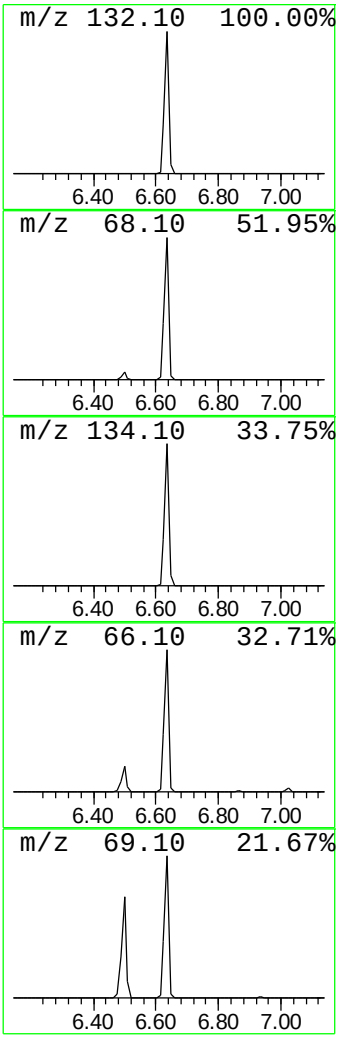
****

Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	106.76 ng	5466950	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082730.D
Acq On : 5 Nov 2015 15:36
Operator : UM/IZ
Sample : G4261-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

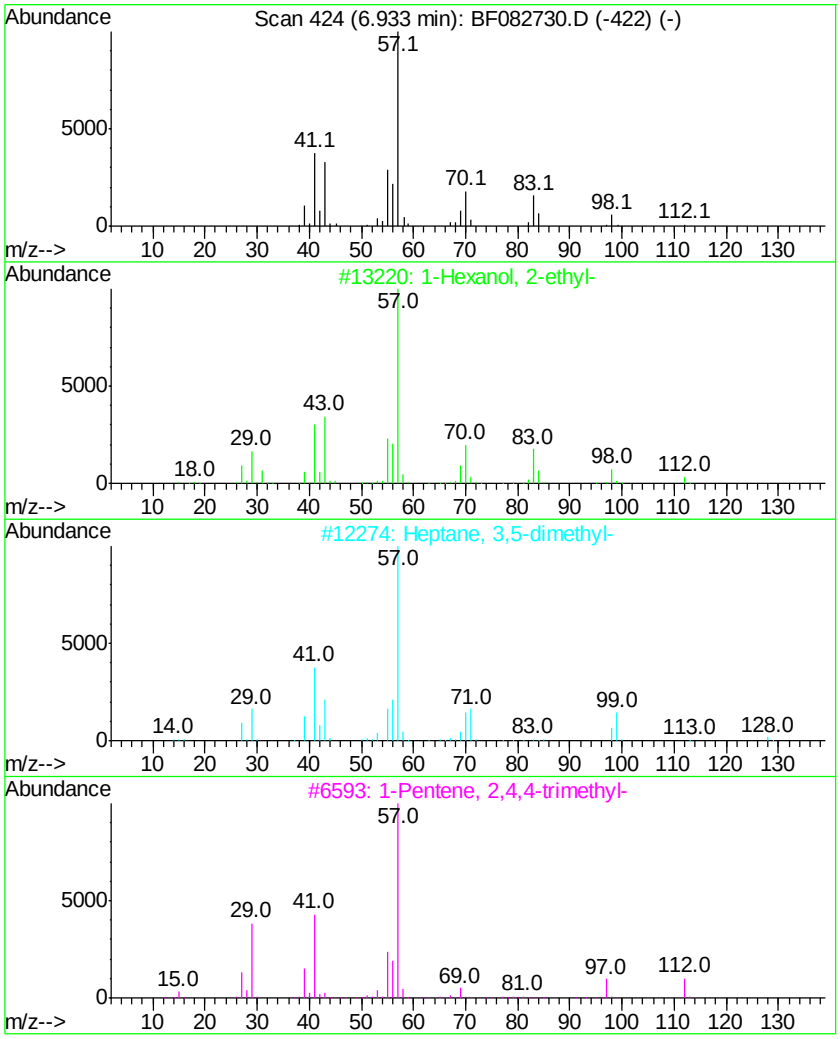
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

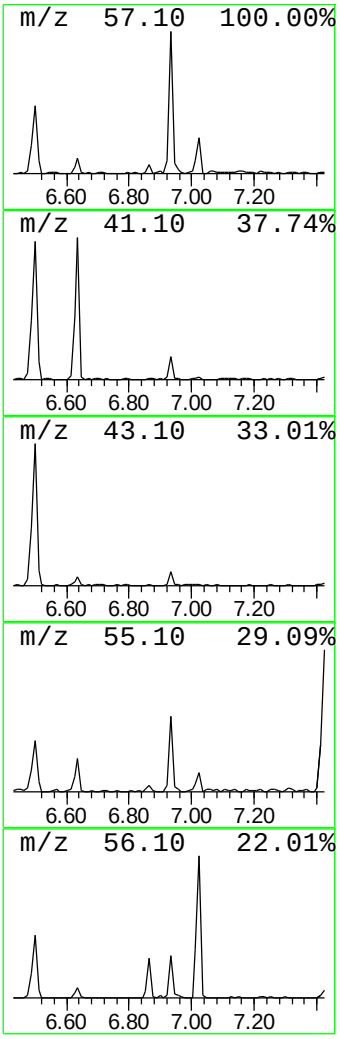
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	2.33 ng	119407	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	59
3	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	47
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	45
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
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Operator : UM/IZ
Sample : G4261-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
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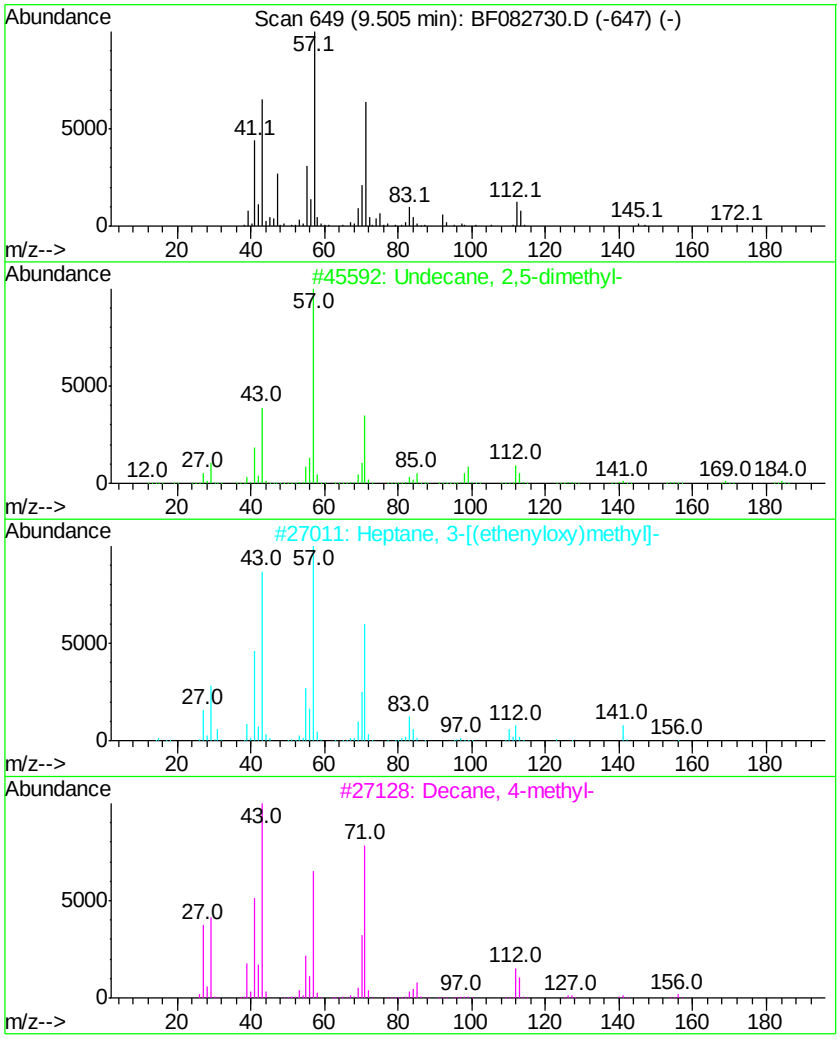
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

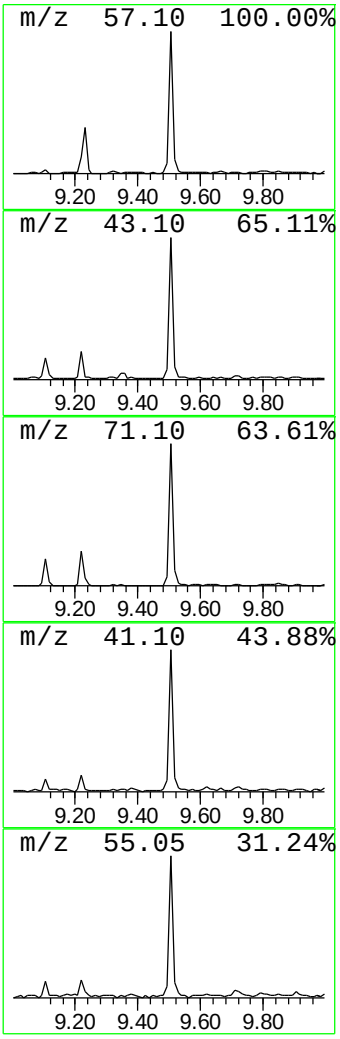
****

Peak Number 7 Undecane, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	5.11 ng	359159	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	53
2	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	50
3	Decane, 4-methyl-	156	C11H24	002847-72-5	50
4	Octane, 3-ethyl-	142	C10H22	005881-17-4	50
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	50





Library Search Compound Report

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Operator : UM/IZ
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

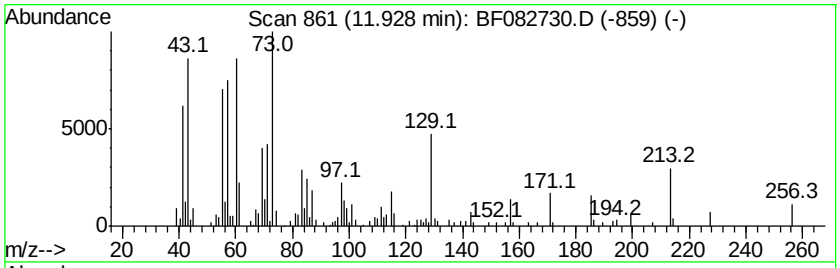
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

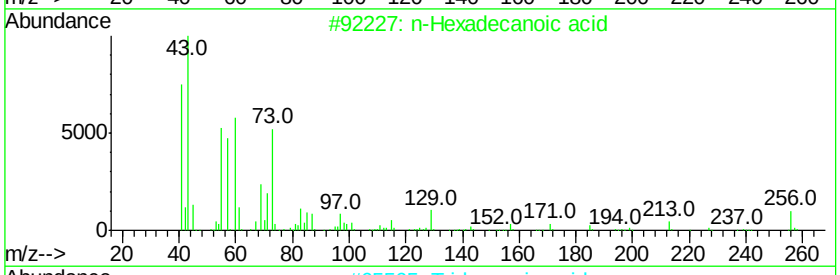
****

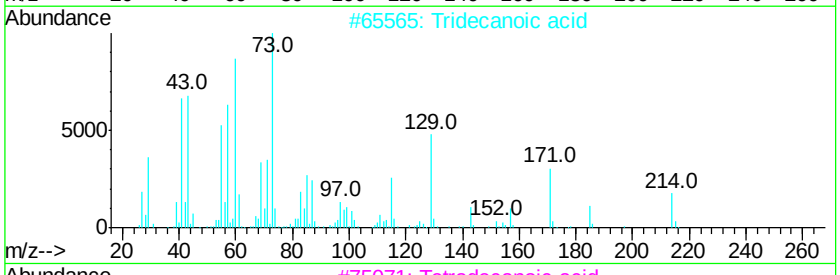
Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

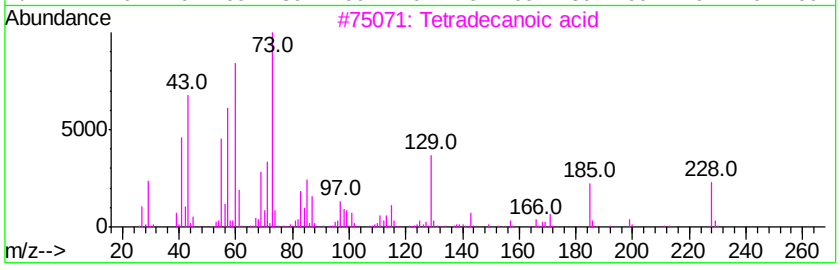
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.05 ng	274524	Phenanthrene-d10	11.39

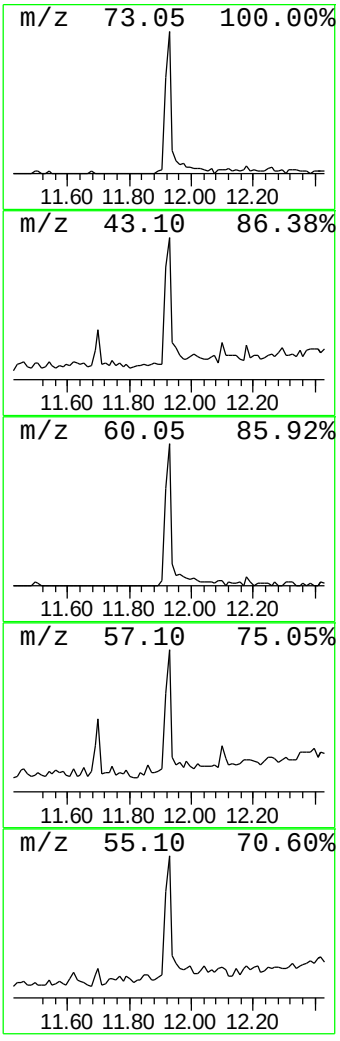
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38











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Sample : G4261-04
Misc :
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Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

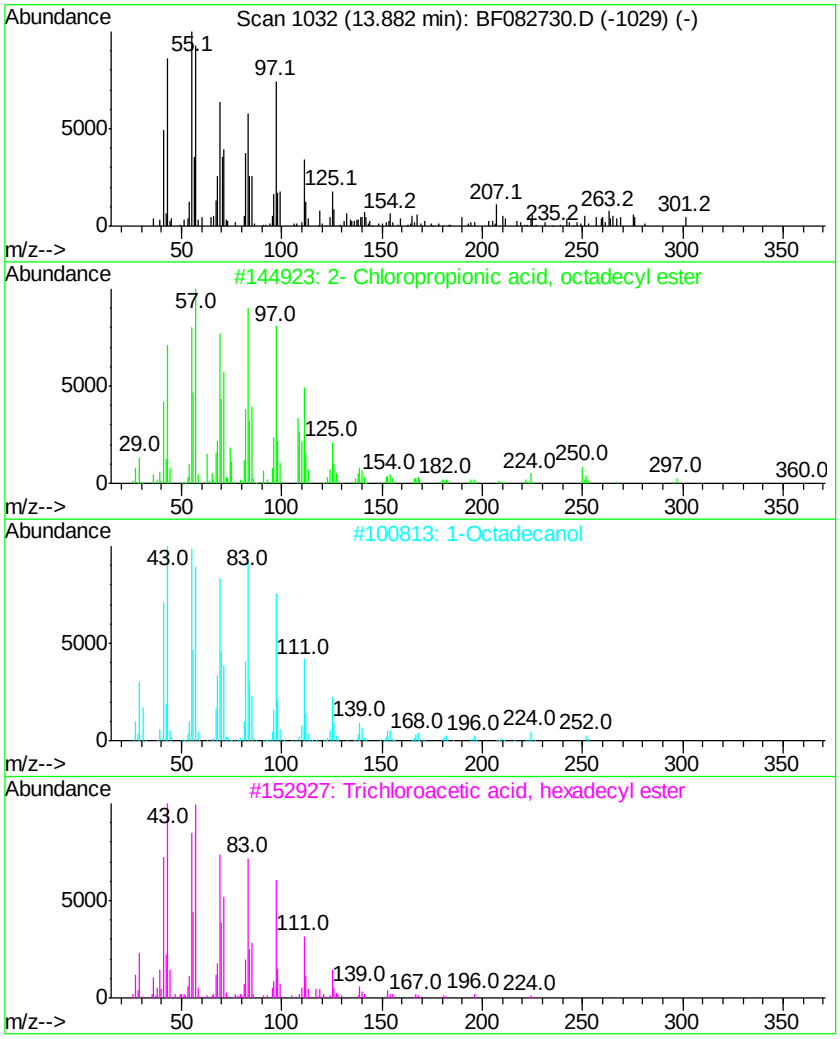
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

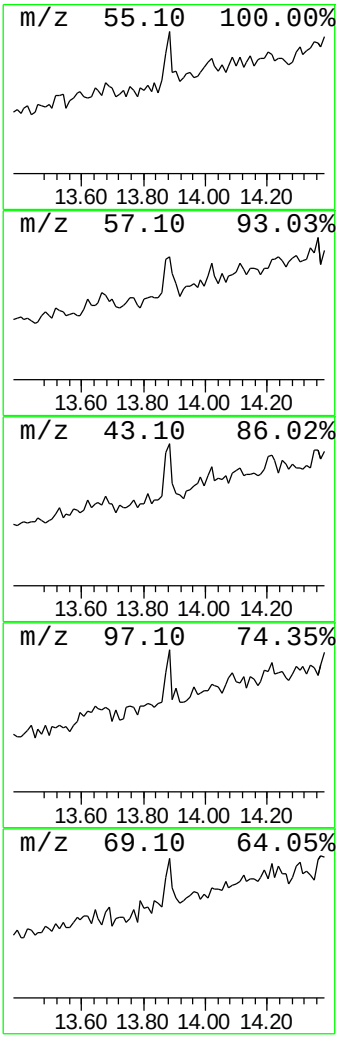
****

Peak Number 10 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.78 ng	150371	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
2	1-Octadecanol	270	C18H38O	000112-92-5	89
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	83
5	1-Nonadecene	266	C19H38	018435-45-5	83





Tentatively Identified Compound (LSC) summary

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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
1,1,3-Trimethoxyp...	2.13	6.0	ng	309766	1	6.86	1024130	20.0
2-Pentanone, 4-hy...	5.06	52.8	ng	2703660	1	6.86	1024130	20.0
unknown6.64	6.64	106.8	ng	5466950	1	6.86	1024130	20.0
1-Hexanol, 2-ethyl-	6.93	2.3	ng	119407	1	6.86	1024130	20.0
Undecane, 2,5-dim...	9.50	5.1	ng	359159	3	9.90	1406820	20.0
n-Hexadecanoic acid	11.93	4.0	ng	274524	4	11.39	1354900	20.0
2- Chloropropioni...	13.88	2.8	ng	150371	5	14.02	1083250	20.0