LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082740.D
Acq On : 5 Nov 2015 20:29
Operator : UM/IZ
Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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:\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	5.047	255	259	267	rVB	1439008	1863889	39.00%	5.272%
2	5.470	293	296	298	rBV	4038874	3927778	82.18%	11.109%
3	6.499	383	386	388	rBV	4098762	4311599	90.21%	12.195%
4	6.636	395	398	400	rBV	4159342	4369796	91.43%	12.359%
5	6.865	416	418	420	rBV	598547	491394	10.28%	1.390%
6	6.933	422	424	429	rVV	96118	83425	1.75%	0.236%
7	7.025	429	432	434	rBV	3713300	3389777	70.92%	9.588%
8	7.425	464	467	469	rBV	2625765	2493716	52.18%	7.053%
9	8.145	528	530	533	rBV	513269	555095	11.61%	1.570%
10	9.231	622	625	627	rBV	5468632	4779521	100.00%	13.518%
11	9.505	647	649	651	rBV	167877	135022	2.83%	0.382%
12	9.619	657	659	661	rBV	834793	685757	14.35%	1.940%
13	9.905	681	684	686	rBV	759018	649298	13.59%	1.836%
14	10.316	718	720	724	rVB2	50734	70188	1.47%	0.199%
15	10.694	750	753	755	rBV	2073257	2500908	52.33%	7.073%
16	10.819	762	764	768	rVB	42201	52662	1.10%	0.149%
17	11.379	811	813	816	rVB2	474704	549425	11.50%	1.554%
18	11.916	858	860	865	rBV2	98790	127413	2.67%	0.360%
19	12.968	950	952	955	rBV	2613623	3273771	68.50%	9.259%
20	13.882	1029	1032	1039	rBV	105713	177522	3.71%	0.502%
21	14.020	1041	1044	1046	rBV	499149	466317	9.76%	1.319%
22	15.448	1166	1169	1172	rBV	320863	401887	8.41%	1.137%

Sum of corrected areas: 35356160

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082740.D
Acq On : 5 Nov 2015 20:29
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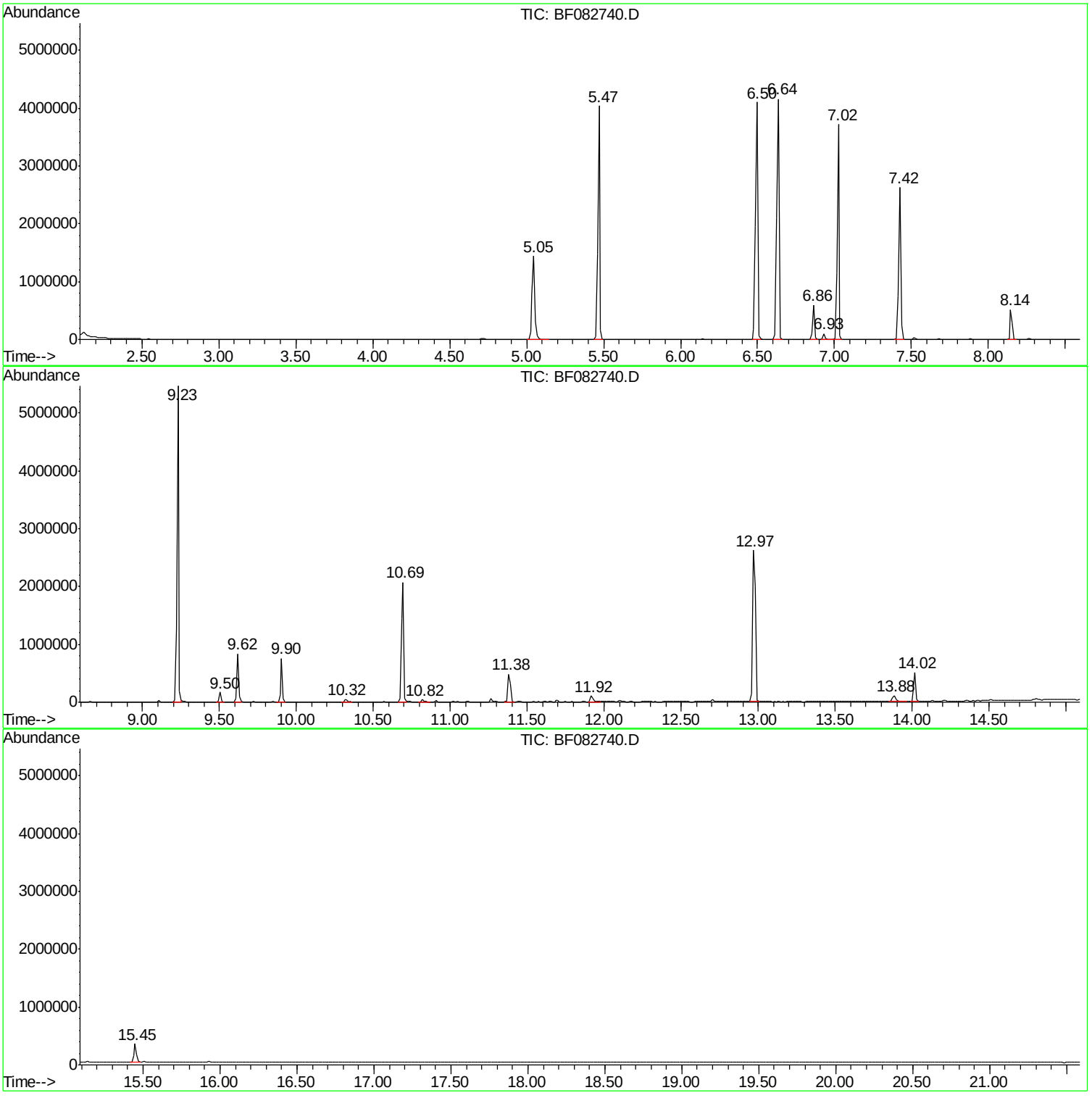
Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5

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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082740.D
Acq On : 5 Nov 2015 20:29
Operator : UM/IZ
Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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

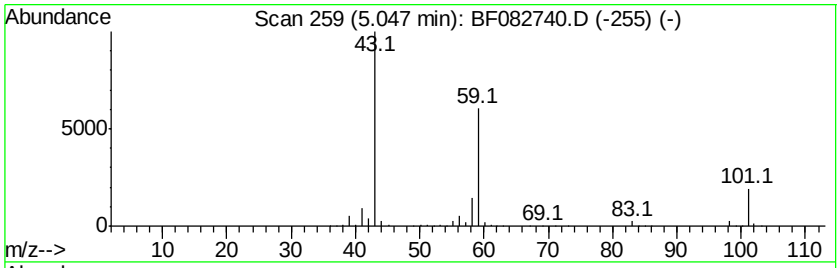
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

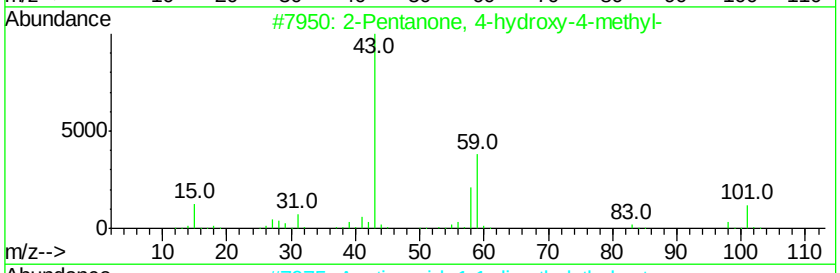
****

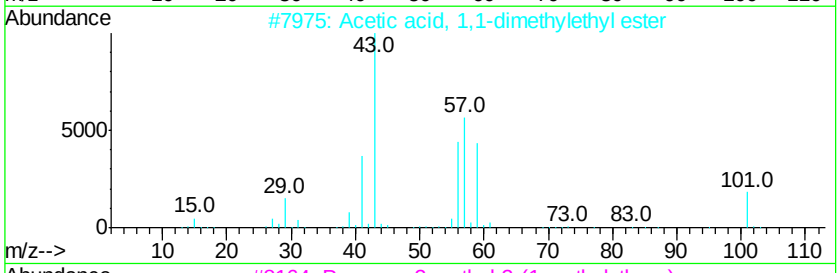
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

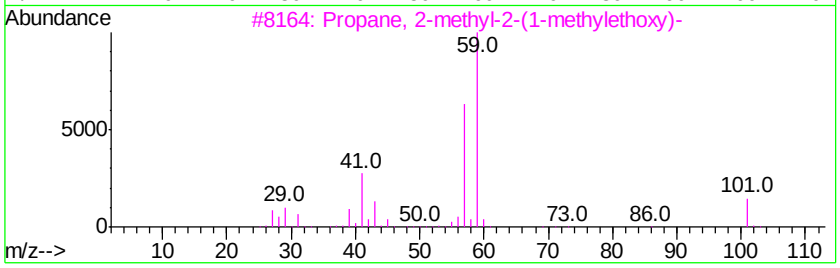
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	75.86 ng	1863890	1,4-Dichlorobenzene-d4	6.86

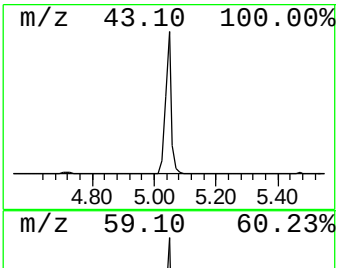
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25

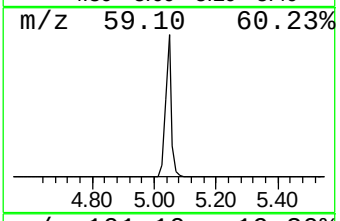


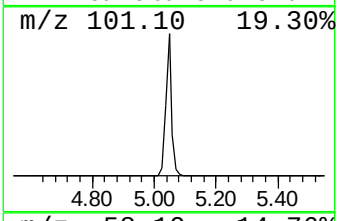


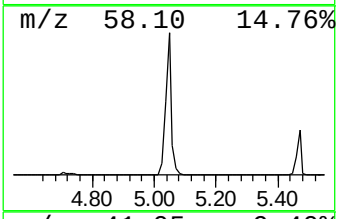


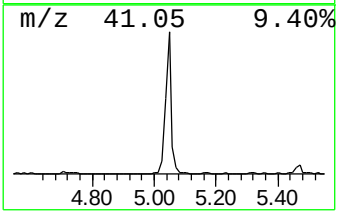












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Data File : BF082740.D
Acq On : 5 Nov 2015 20:29
Operator : UM/IZ
Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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

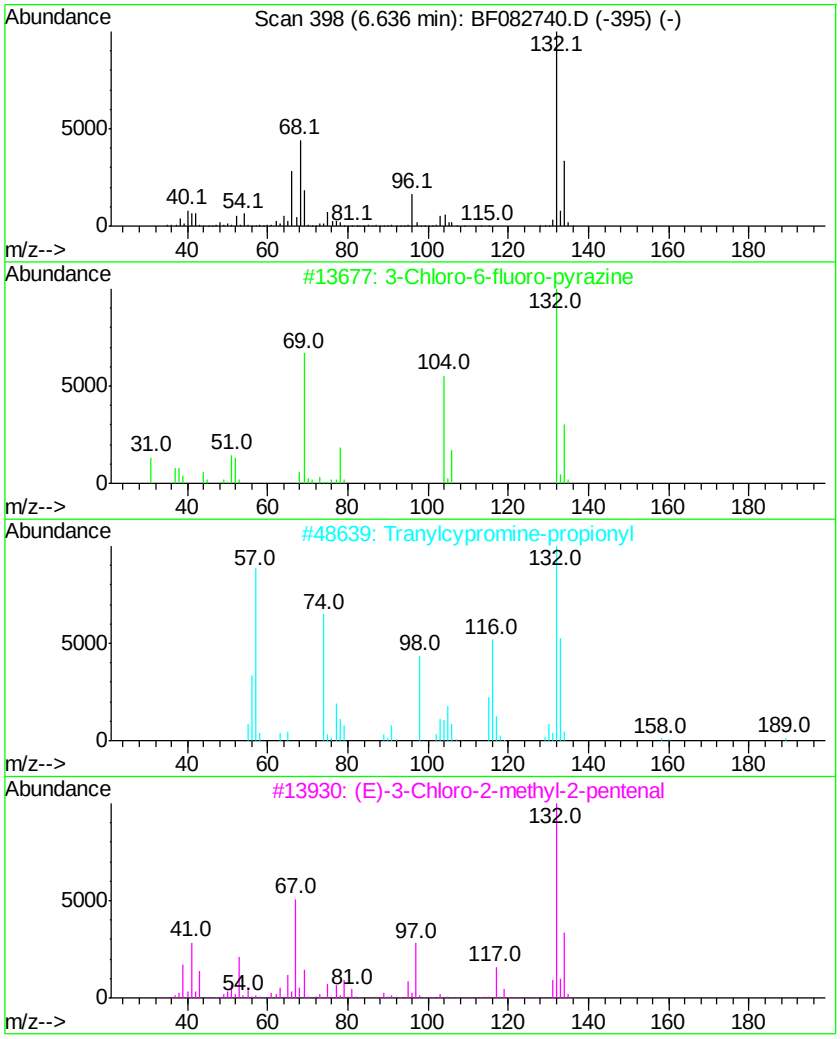
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

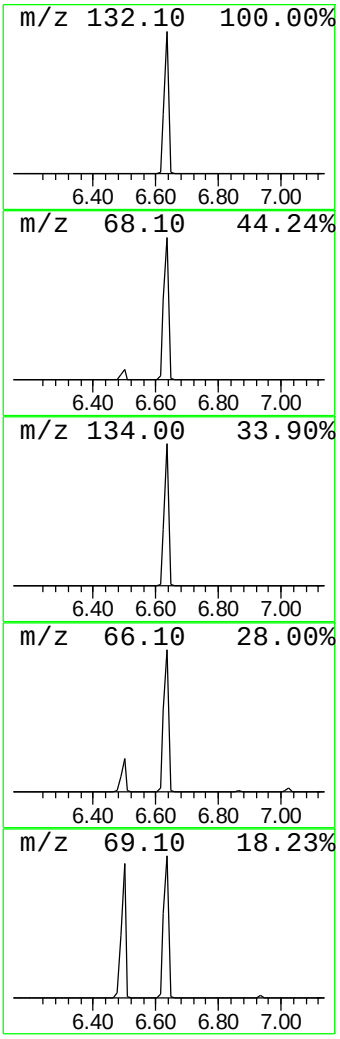
****

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	177.85 ng	4369800	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Sample : G4261-10
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Instrument : BNA_F
ClientSampleId : SB-5

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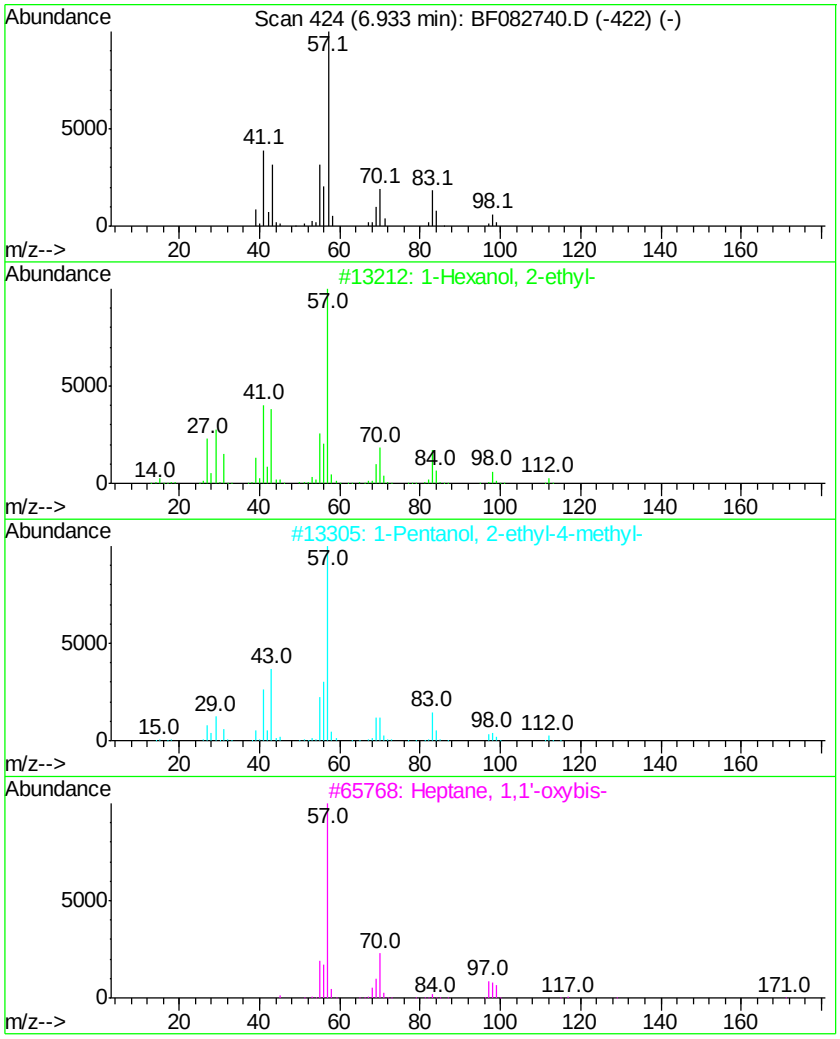
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

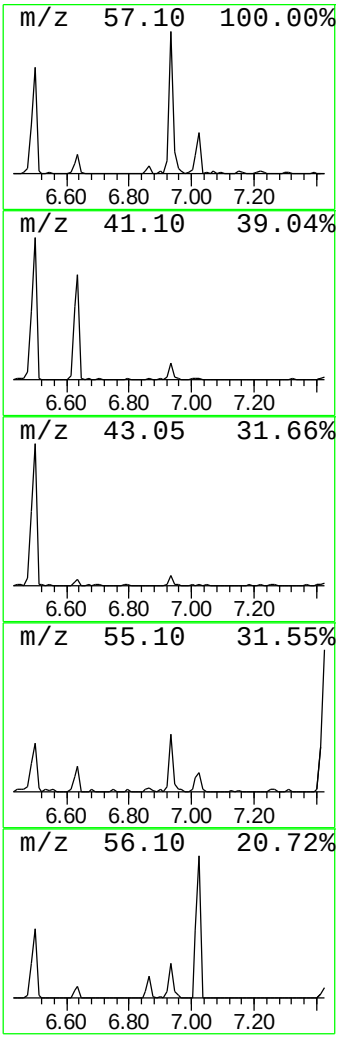
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	3.40 ng	83425	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	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082740.D
Acq On : 5 Nov 2015 20:29
Operator : UM/IZ
Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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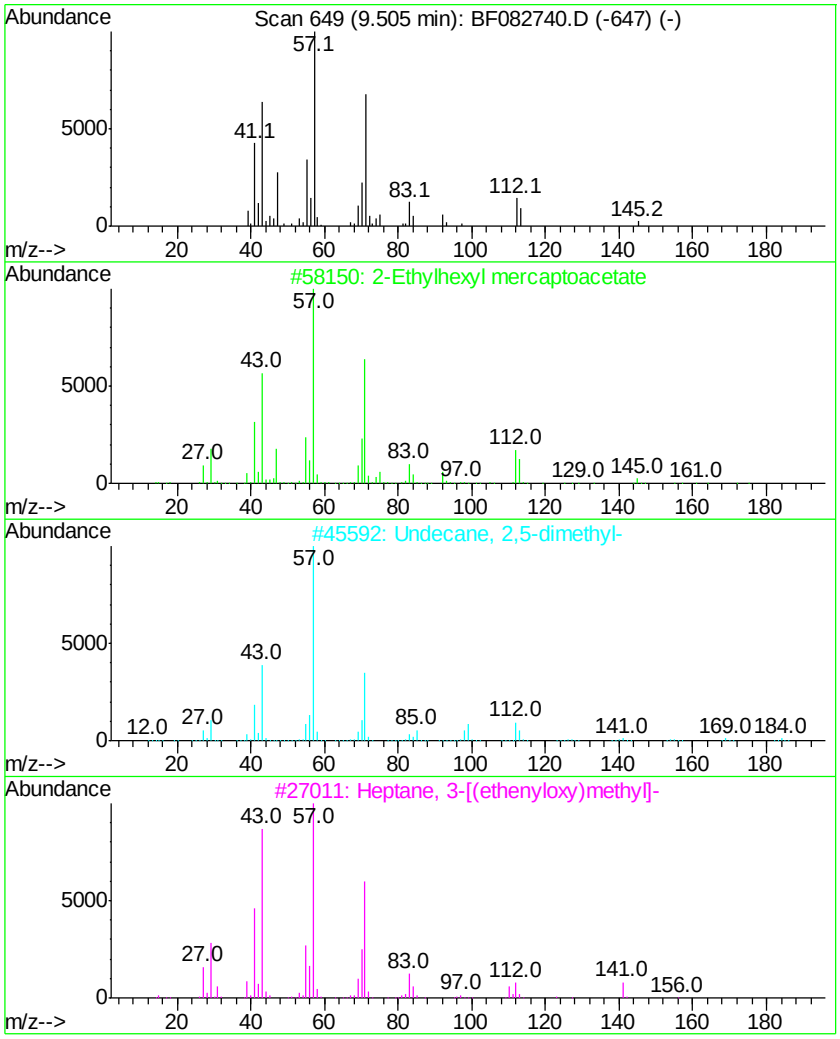
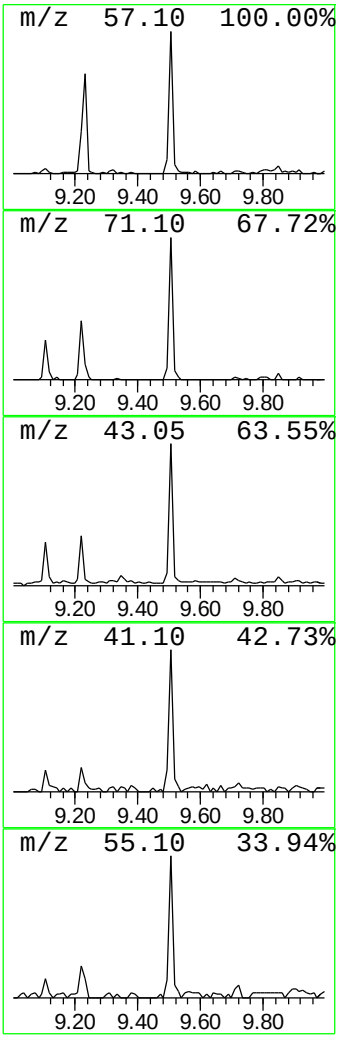
****

Peak Number 5 2-Ethylhexyl mercaptoacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	4.16 ng	135022	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	86
2	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	58
3	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	53
4	Decane, 4-methyl-	156	C11H24	002847-72-5	50
5	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	50





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Sample : G4261-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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

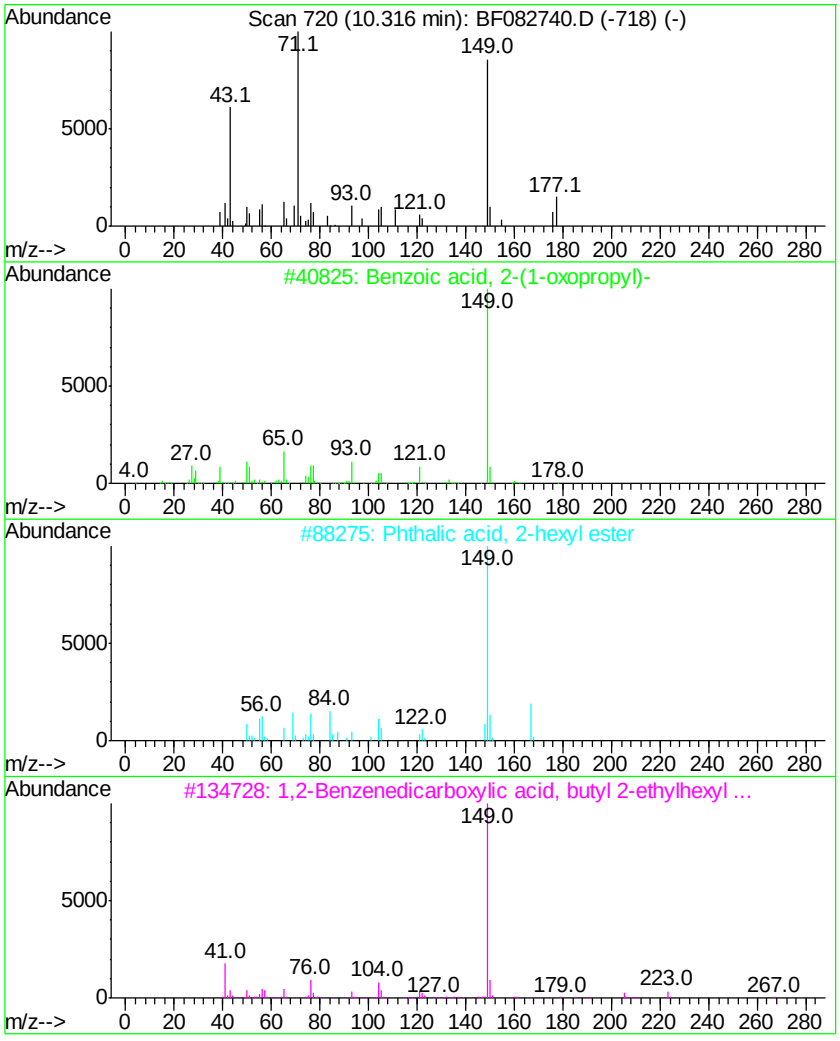
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

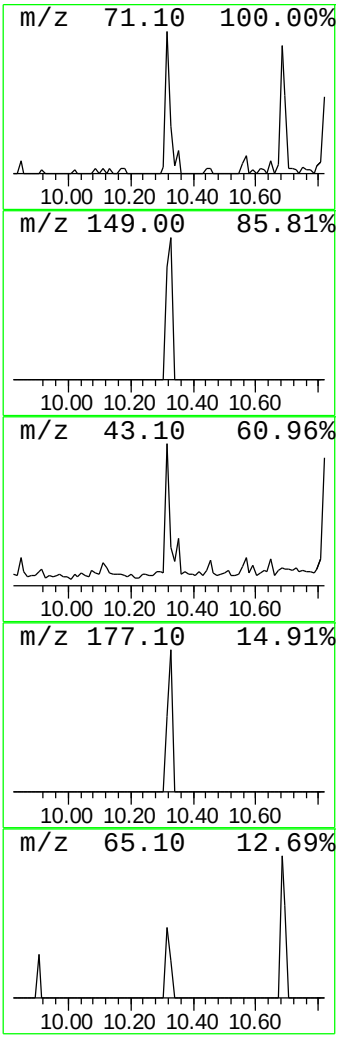
****

Peak Number 6 unknown10.32 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.16 ng	70188	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(1-oxopropyl)-	178	C10H10O3	002360-45-4	38
2	Phthalic acid, 2-hexyl ester	250	C14H18O4	079107-80-5	38
3	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	38
4	2-Acetylbenzoic acid	164	C9H8O3	000577-56-0	38
5	1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	37





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Instrument : BNA_F
ClientSampleId : SB-5

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

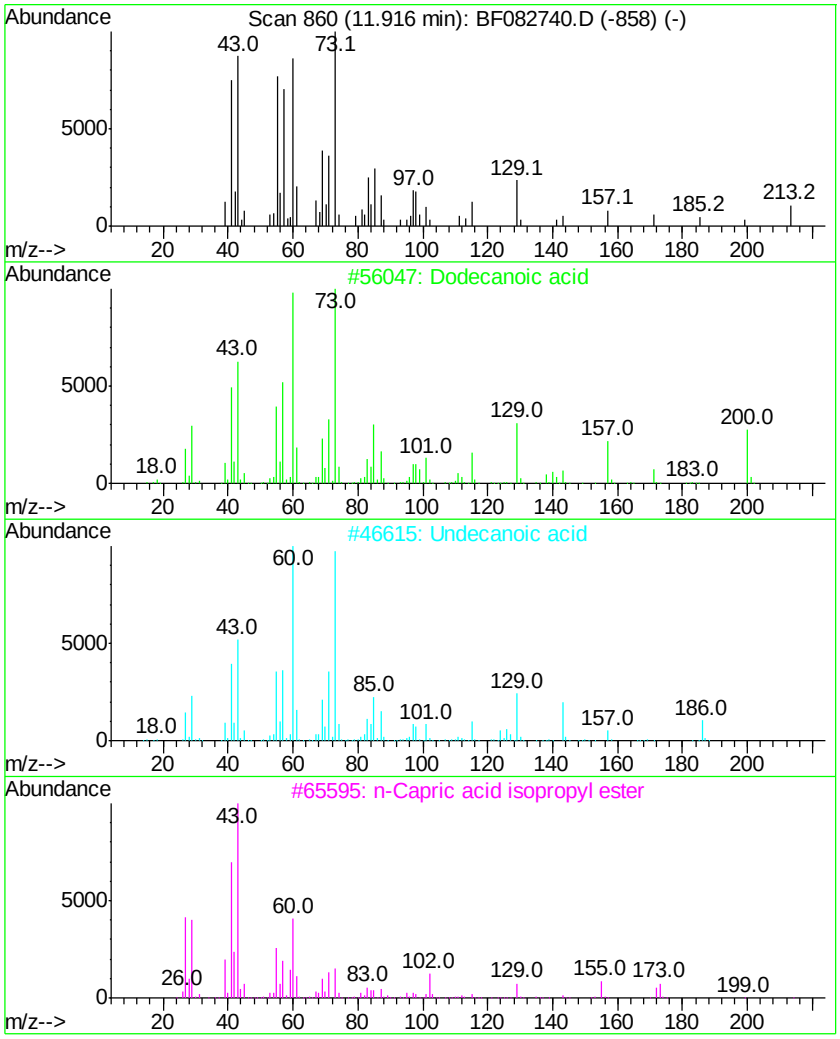
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

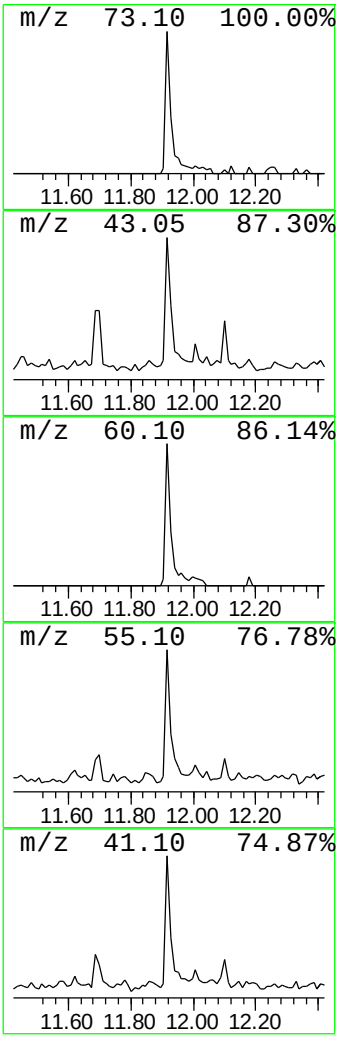
****

Peak Number 7 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.64 ng	127413	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	86
2	Undecanoic acid	186	C11H22O2	000112-37-8	78
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
4	Nonanoic acid	158	C9H18O2	000112-05-0	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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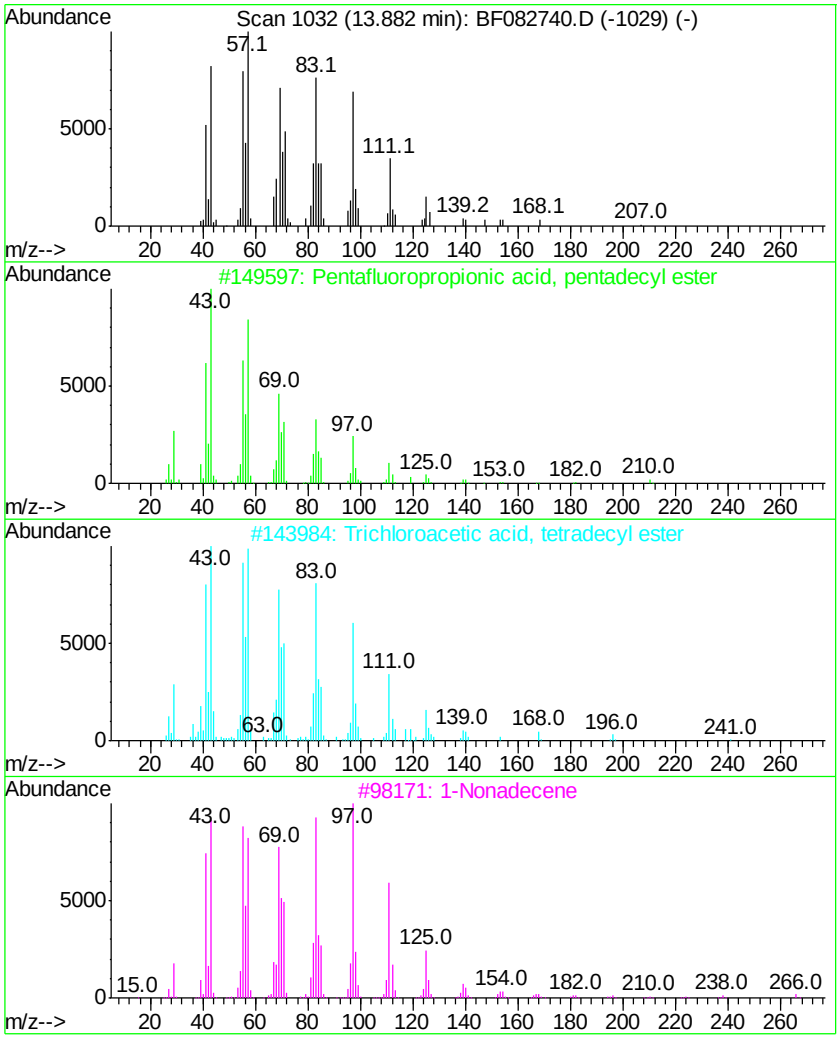
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

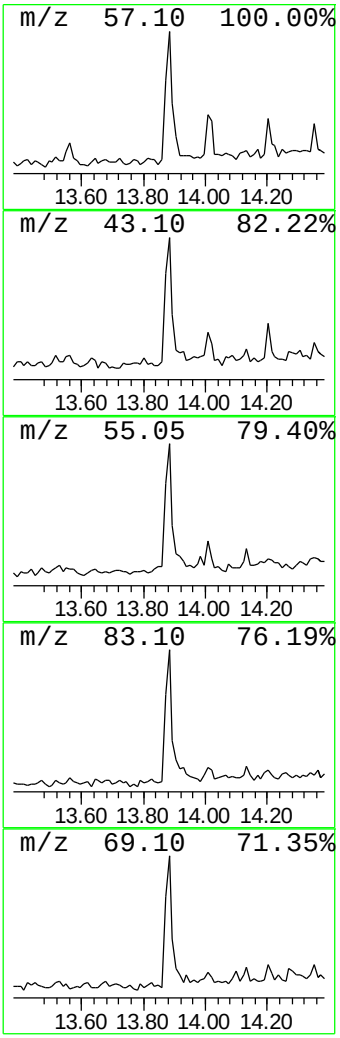
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.61 ng	177522	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90





Tentatively Identified Compound (LSC) summary

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Acq On : 5 Nov 2015 20:29
Operator : UM/IZ
Sample : G4261-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	75.9	ng	1863890	1	6.86	491394	20.0
unknown6.64	6.64	177.8	ng	4369800	1	6.86	491394	20.0
1-Hexanol, 2-ethyl-	6.93	3.4	ng	83425	1	6.86	491394	20.0
2-Ethylhexyl merc...	9.50	4.2	ng	135022	3	9.90	649298	20.0
unknown10.32	10.32	2.2	ng	70188	3	9.90	649298	20.0
Dodecanoic acid	11.92	4.6	ng	127413	4	11.38	549425	20.0
Pentafluoropropio...	13.88	7.6	ng	177522	5	14.02	466317	20.0