LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

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-BF123115.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	2.167	5	7	19	rVB3	97563	241235	2.20%	0.308%
2	5.081	259	262	267	rVB	990051	1160079	10.59%	1.479%
3	5.493	296	298	301	rVB	3763553	4732341	43.19%	6.033%
4	6.522	386	388	390	rBV	3569783	3038020	27.73%	3.873%
5	6.659	397	400	403	rBV	7818055	7542634	68.85%	9.615%
6	6.887	418	420	422	rBV	2479570	2052877	18.74%	2.617%
7	6.956	424	426	428	rVV	429126	356553	3.25%	0.455%
8	7.047	431	434	436	rVB	8080655	7345697	67.05%	9.364%
9	7.207	446	448	452	rBV2	62152	113734	1.04%	0.145%
10	7.299	452	456	458	rVB	190515	215500	1.97%	0.275%
11	7.459	465	470	472	rBV	6318909	7587464	69.25%	9.672%
12	7.539	475	477	479	rBV	140778	138309	1.26%	0.176%
13	7.882	503	507	508	rBV2	80033	139168	1.27%	0.177%
14	8.087	523	525	526	rVB	106117	133974	1.22%	0.171%
15	8.133	526	529	531	rBV	149480	188194	1.72%	0.240%
16	8.179	531	533	534	rBV	2656564	2664820	24.32%	3.397%
17	9.128	614	616	618	rBV	160107	160182	1.46%	0.204%
18	9.253	624	627	630	rBV	8387498	10955955	100.00%	13.966%
19	9.390	637	639	641	rVB	872613	697499	6.37%	0.889%
20	9.928	684	686	688	rBV	2597396	2809974	25.65%	3.582%
21	10.728	752	756	758	rBV	4911630	7232605	66.02%	9.220%
22	11.413	814	816	818	rVV	3255234	2786882	25.44%	3.553%
23	11.814	848	851	853	rBV2	680084	863869	7.88%	1.101%
24	12.831	937	940	942	rBV	319315	268399	2.45%	0.342%
25	13.014	952	956	958	rBV	7207741	10778810	98.38%	13.741%
26	13.539	999	1002	1004	rBV	143923	178277	1.63%	0.227%
27	14.054	1044	1047	1049	rBV	2117019	2357861	21.52%	3.006%
28	15.494	1170	1173	1175	rBV	1183069	1704622	15.56%	2.173%

Sum of corrected areas: 78445534

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
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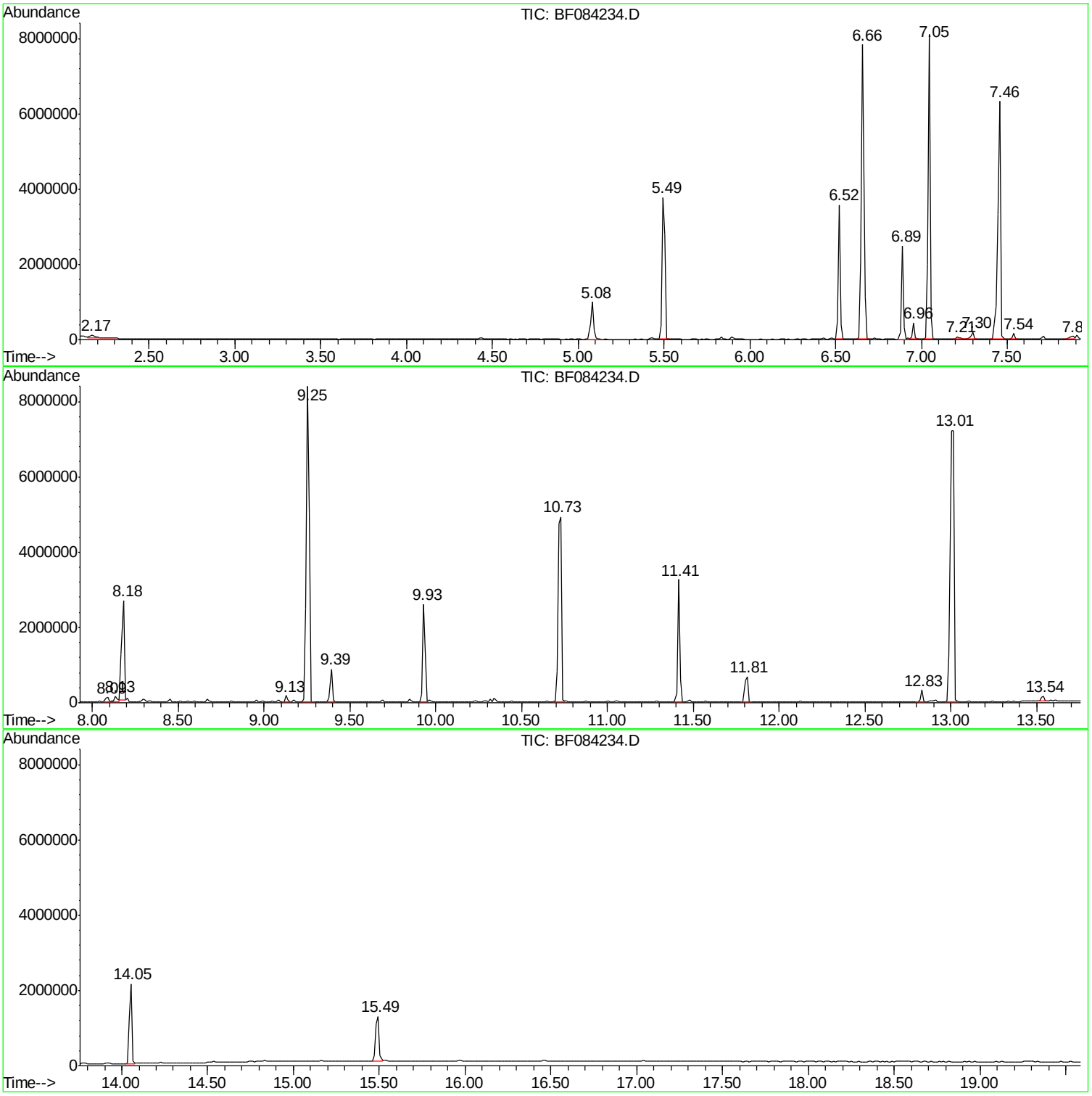
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

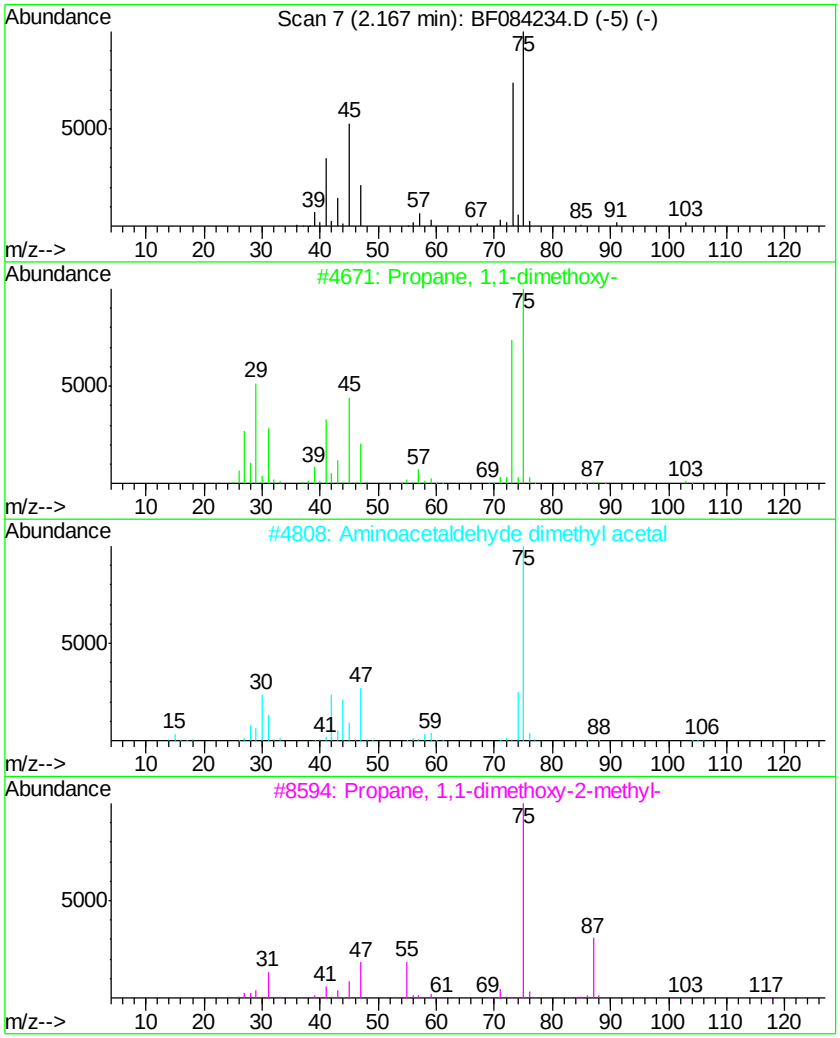
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

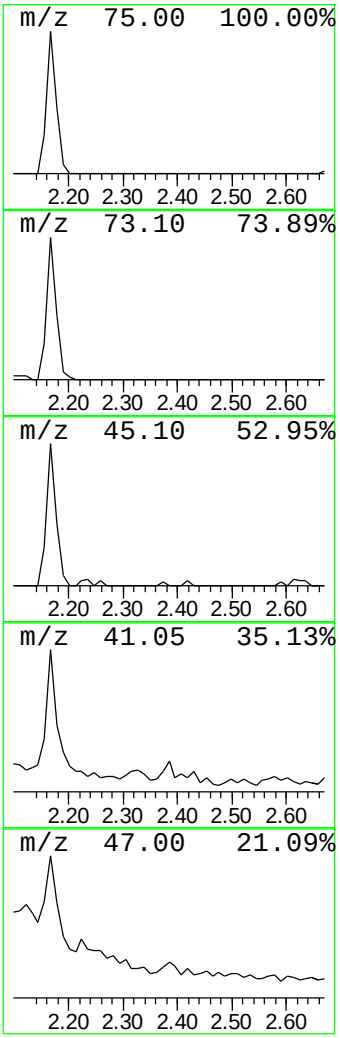
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.35 ng	241235	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
3	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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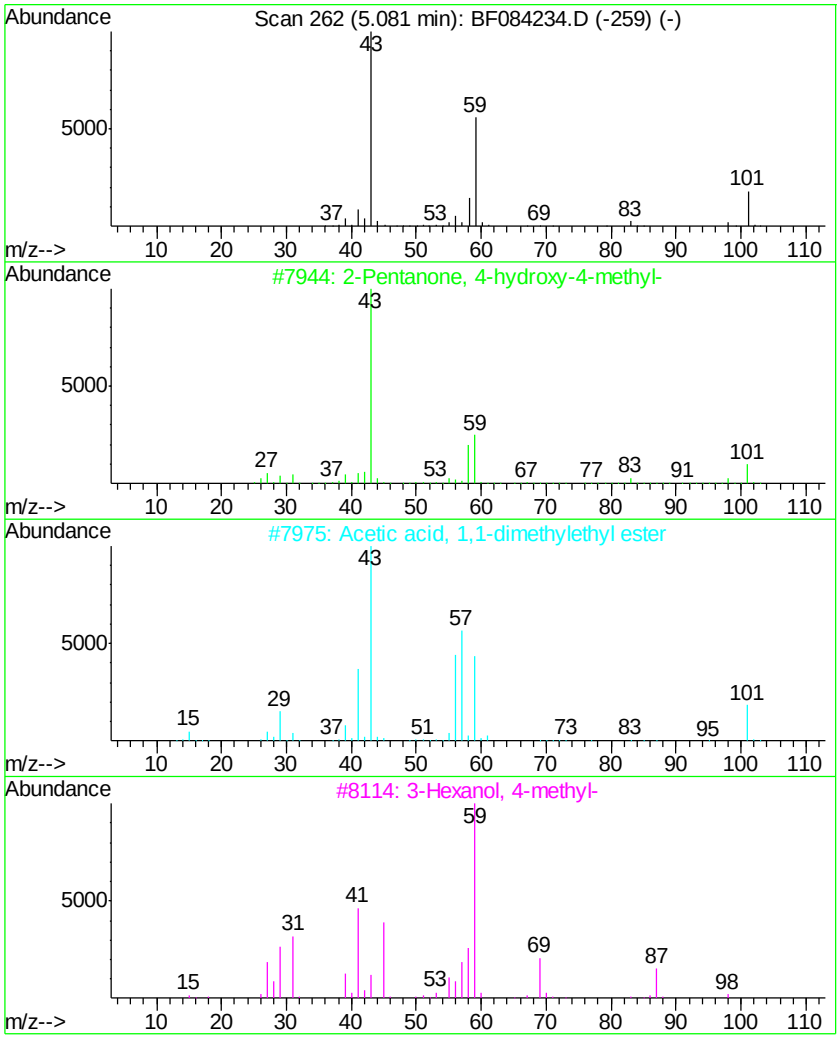
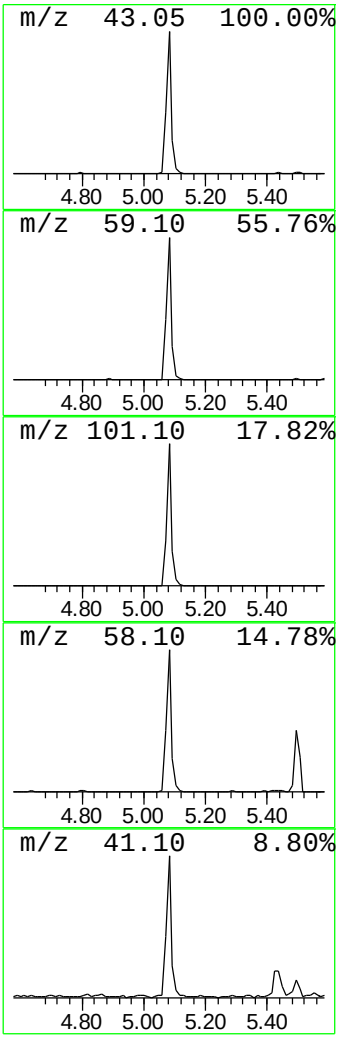
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	11.30 ng	1160080	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

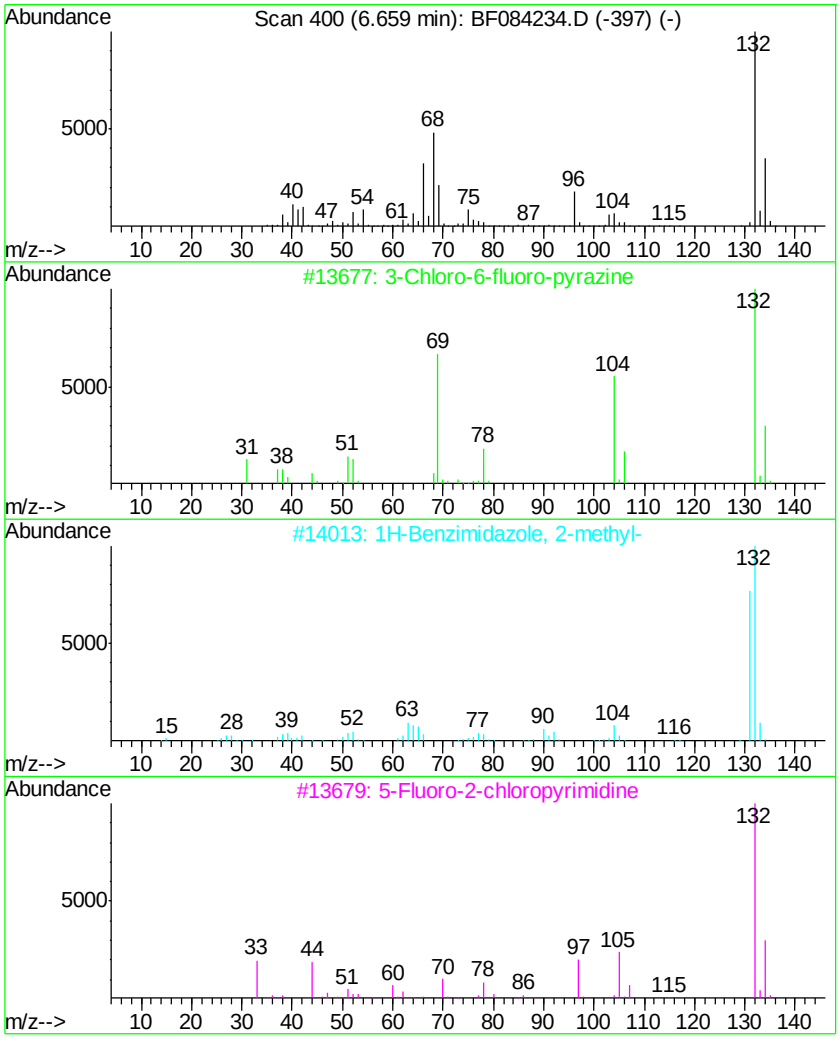
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

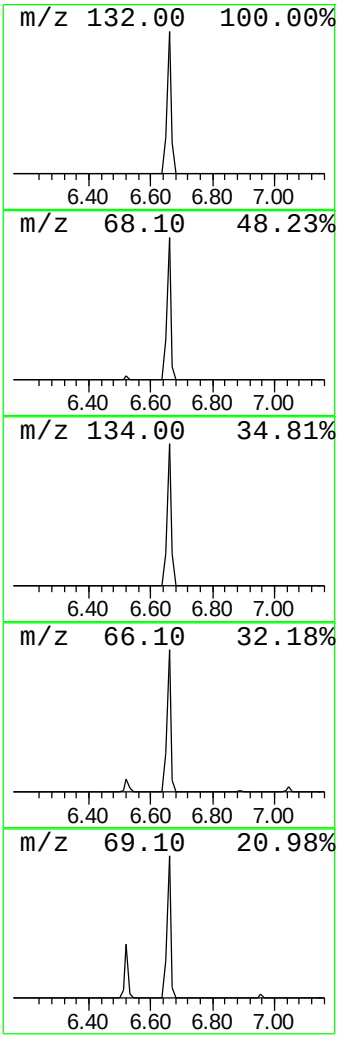
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	73.48 ng	7542630	1,4-Dichlorobenzene-d4	6.89

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	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084234.D
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Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

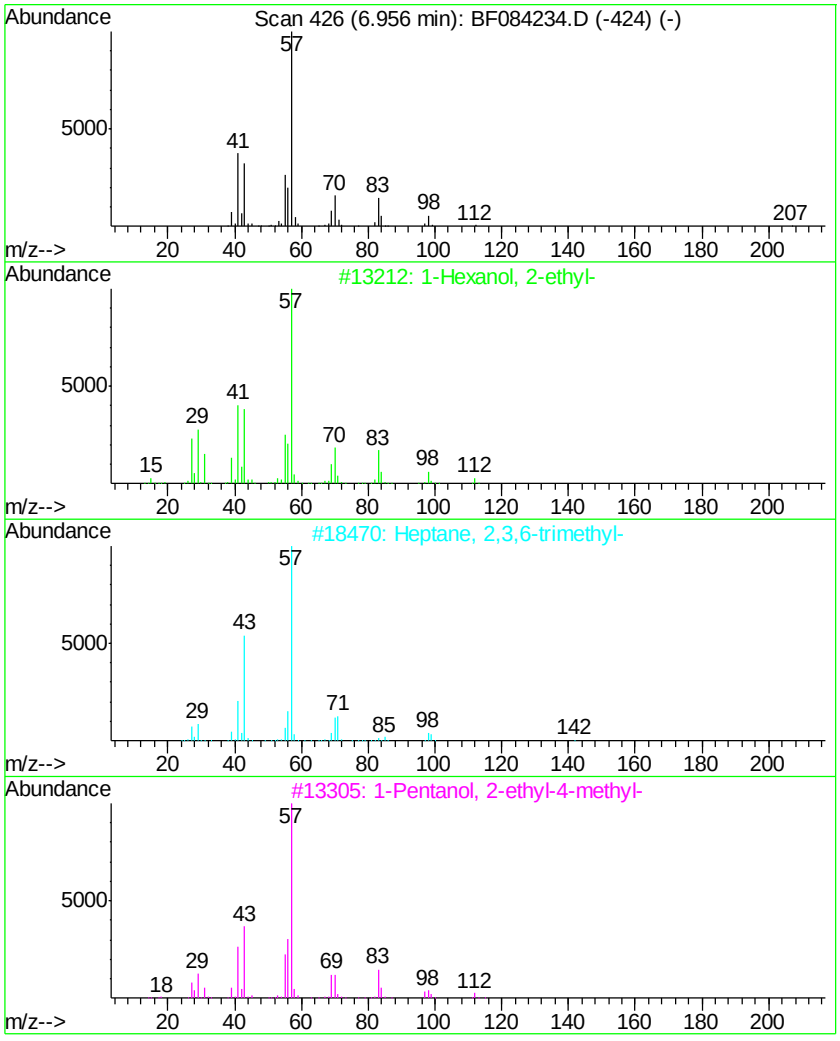
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

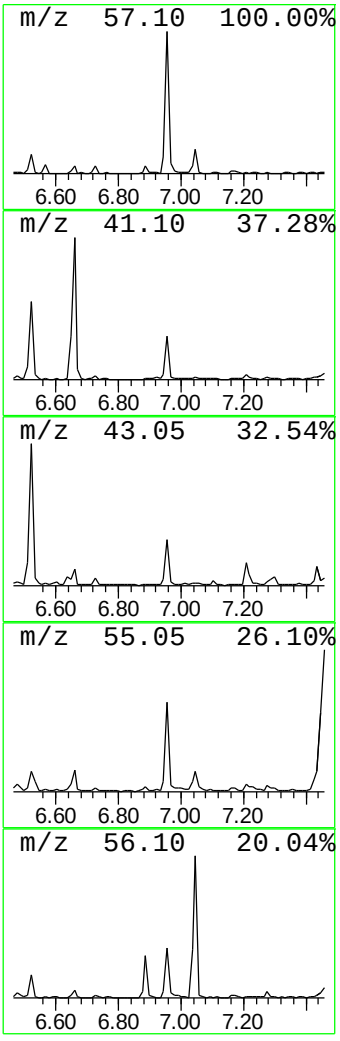
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	3.47 ng	356553	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
5	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

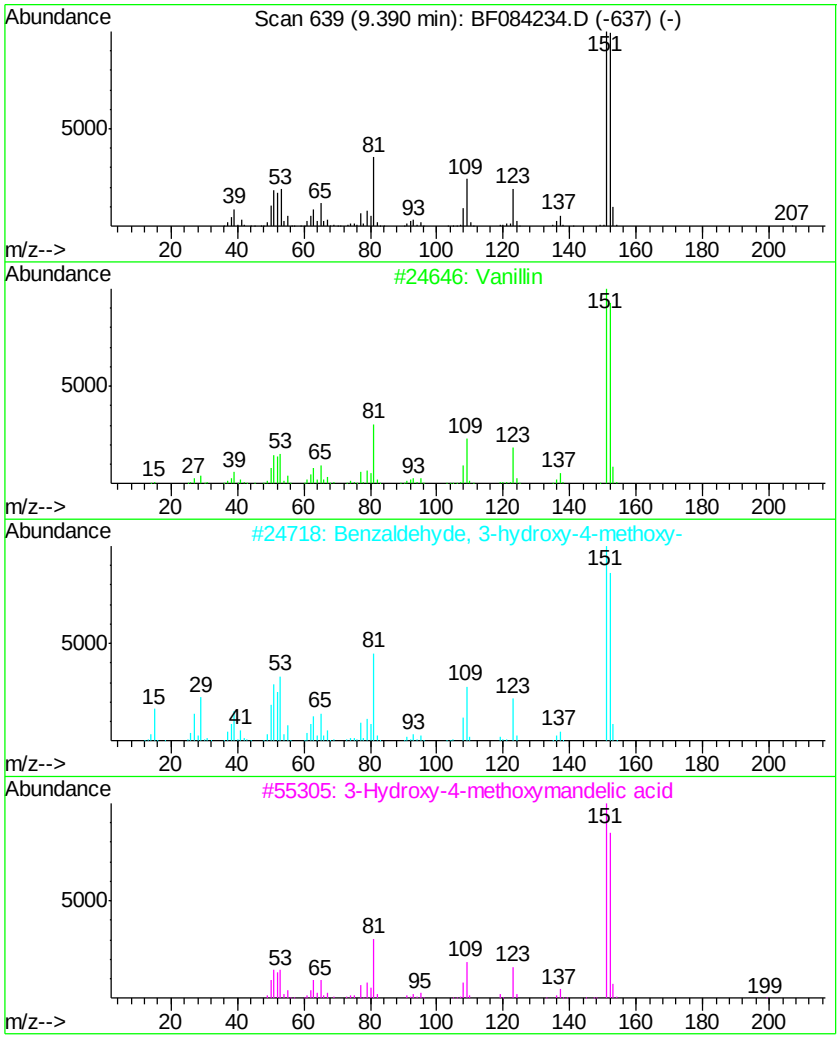
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

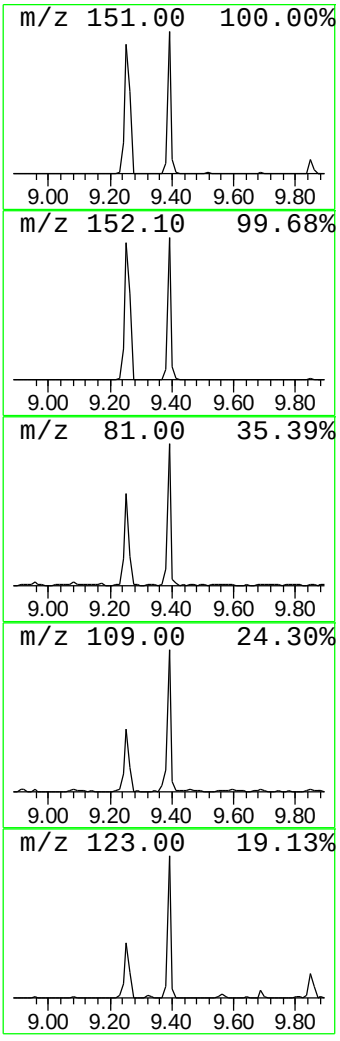
****

Peak Number 7 Vanillin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	4.96 ng	697499	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
3	3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	91
4	4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	81
5	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	59





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Sample : G4982-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EB-S8-2015-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

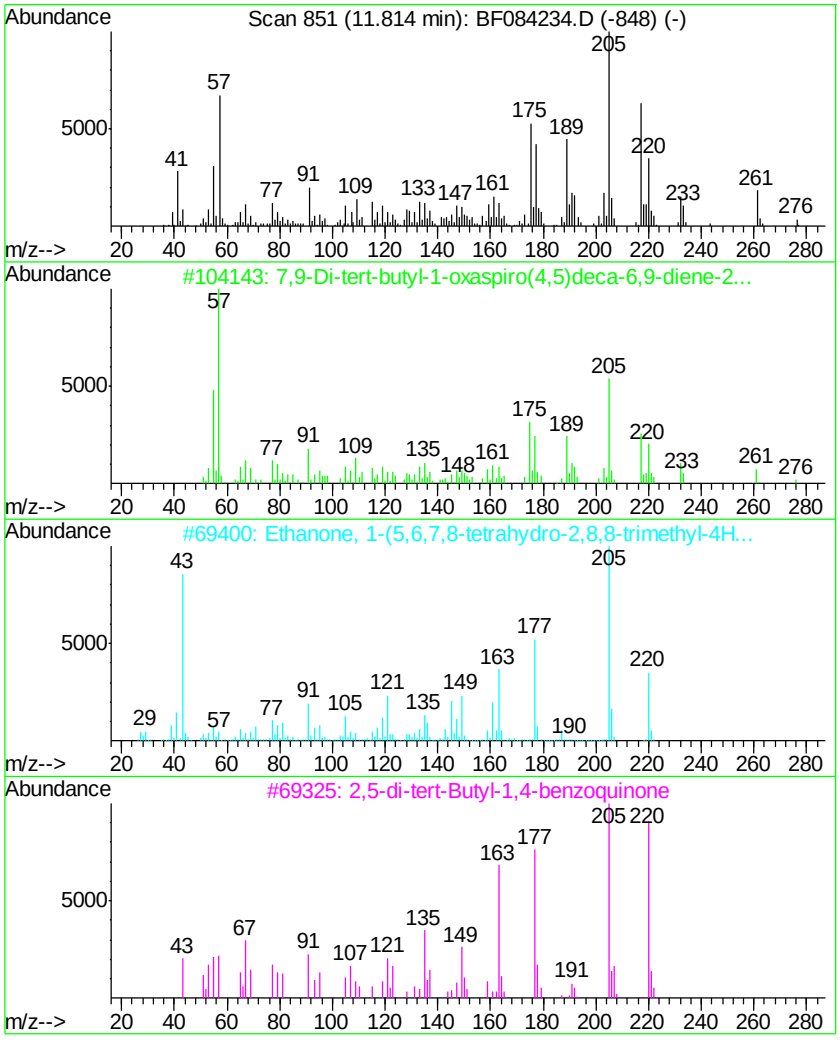
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

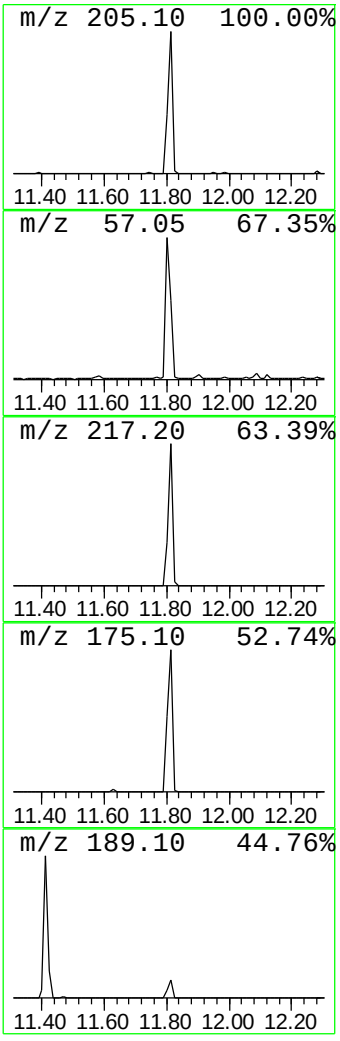
****

Peak Number 8 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	6.20 ng	863869	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	64
3	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	45
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

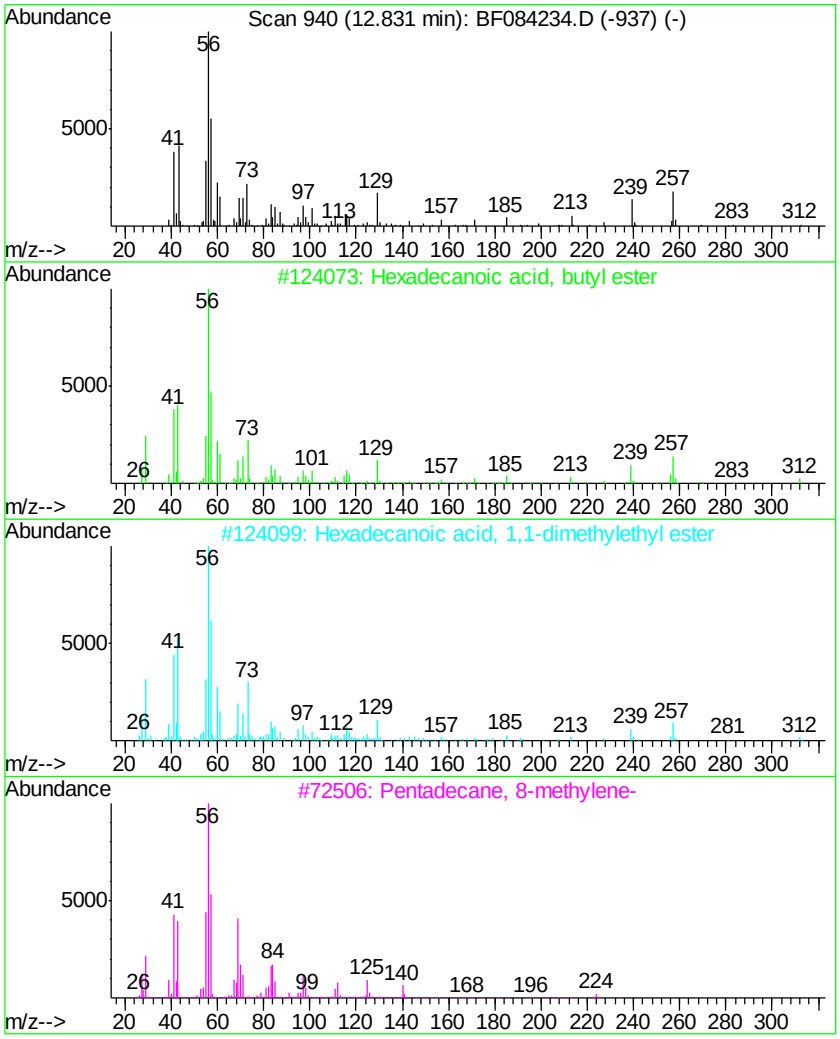
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

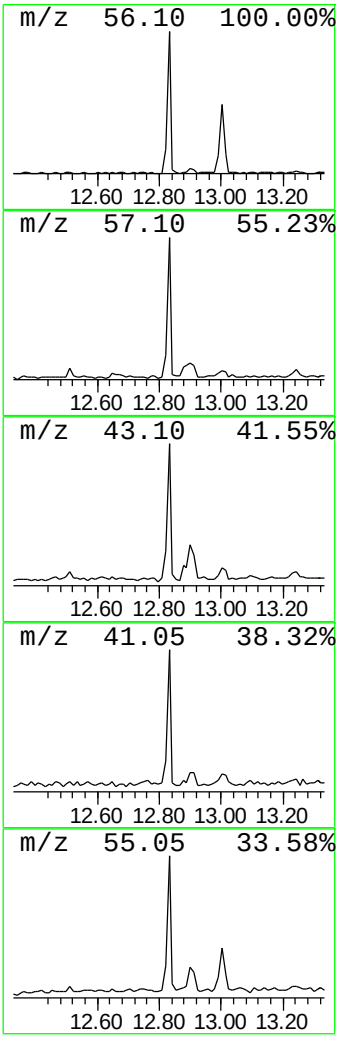
****

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.28 ng	268399	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084234.D
Acq On : 4 Jan 2016 13:04
Operator : UM/SJ
Sample : G4982-02
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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
Propane, 1,1-dime...	2.17	2.4	ng	241235	1	6.89	2052880	20.0
2-Pentanone, 4-hy...	5.08	11.3	ng	1160080	1	6.89	2052880	20.0
unknown6.66	6.66	73.5	ng	7542630	1	6.89	2052880	20.0
1-Hexanol, 2-ethyl-	6.96	3.5	ng	356553	1	6.89	2052880	20.0
Vanillin	9.39	5.0	ng	697499	3	9.93	2809970	20.0
7,9-Di-tert-butyl...	11.81	6.2	ng	863869	4	11.41	2786880	20.0
Hexadecanoic acid...	12.83	2.3	ng	268399	5	14.05	2357860	20.0