LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

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-BF100516.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	3.434	95	96	106	rBV	69556	170857	3.11%	0.338%
2	5.194	247	250	253	rBV	1457979	1678246	30.50%	3.317%
3	5.606	283	286	288	rBV	3229491	4367572	79.38%	8.632%
4	6.612	371	374	377	rBV	4275202	4429940	80.52%	8.756%
5	6.760	384	387	389	rBV	5163438	4659143	84.68%	9.209%
6	6.989	405	407	410	rBV	1218234	1287086	23.39%	2.544%
7	7.149	419	421	424	rVB	4121474	3603609	65.50%	7.122%
8	7.549	454	456	459	rBV	2329208	3097471	56.30%	6.122%
9	8.280	518	520	522	rBV	2172898	1860072	33.81%	3.676%
10	9.366	612	615	617	rBV	4510739	5501901	100.00%	10.874%
11	9.755	646	649	651	rBV	1890393	1582016	28.75%	3.127%
12	10.040	672	674	676	rVB	2219042	1991138	36.19%	3.935%
13	10.475	711	712	714	rVB	83802	58981	1.07%	0.117%
14	10.829	740	743	746	rBV	2744375	2646165	48.10%	5.230%
15	10.955	752	754	758	rBV2	62108	113806	2.07%	0.225%
16	11.401	790	793	794	rBV	88476	84156	1.53%	0.166%
17	11.538	802	805	807	rBV	1773087	2117030	38.48%	4.184%
18	11.755	821	824	828	rBV	94673	135925	2.47%	0.269%
19	12.052	848	850	853	rBV2	247480	342173	6.22%	0.676%
20	12.749	908	911	913	rBV	283044	275788	5.01%	0.545%
21	12.841	918	919	923	rBV2	178051	264303	4.80%	0.522%
22	12.978	927	931	932	rBV	260340	259241	4.71%	0.512%
23	13.126	941	944	946	rVB	6070304	5423046	98.57%	10.718%
24	13.355	963	964	967	rVB2	47119	62720	1.14%	0.124%
25	14.018	1020	1022	1028	rVB	268155	375265	6.82%	0.742%
26	14.178	1033	1036	1042	rVB	1974817	2126597	38.65%	4.203%
27	14.658	1075	1078	1082	rBV3	64035	137680	2.50%	0.272%
28	15.241	1126	1129	1134	rBV	97521	223433	4.06%	0.442%
29	15.321	1134	1136	1138	rBV	34886	66636	1.21%	0.132%
30	15.550	1153	1156	1159	rVB	66244	89219	1.62%	0.176%
31	15.607	1159	1161	1164	rBV	69264	113203	2.06%	0.224%
32	15.675	1164	1167	1170	rBV	821989	1324055	24.07%	2.617%
33	17.184	1296	1299	1305	rVB2	29916	64627	1.17%	0.128%
34	17.630	1335	1338	1347	rVB	25796	62881	1.14%	0.124%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

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-BF100516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 50595981

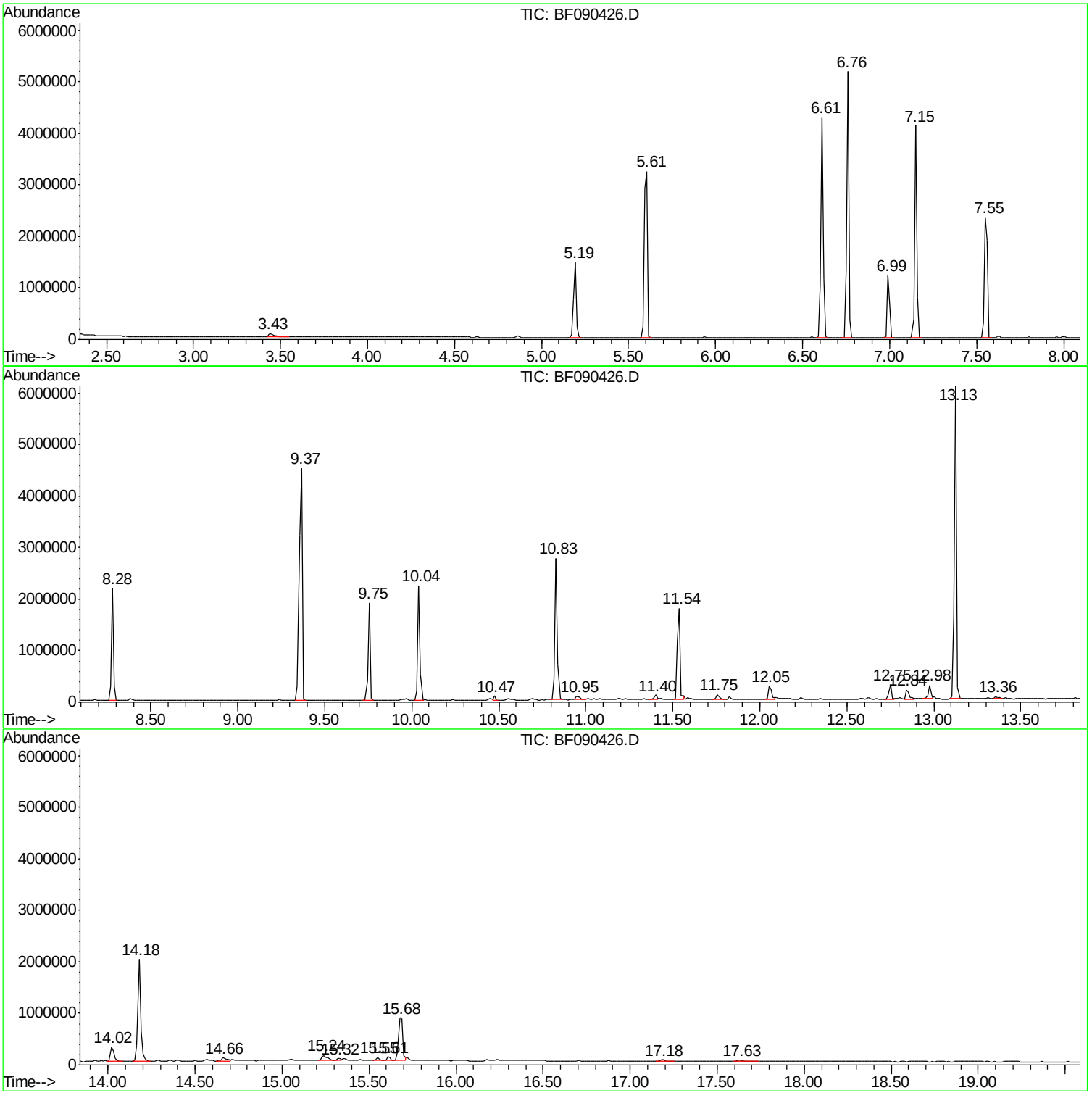
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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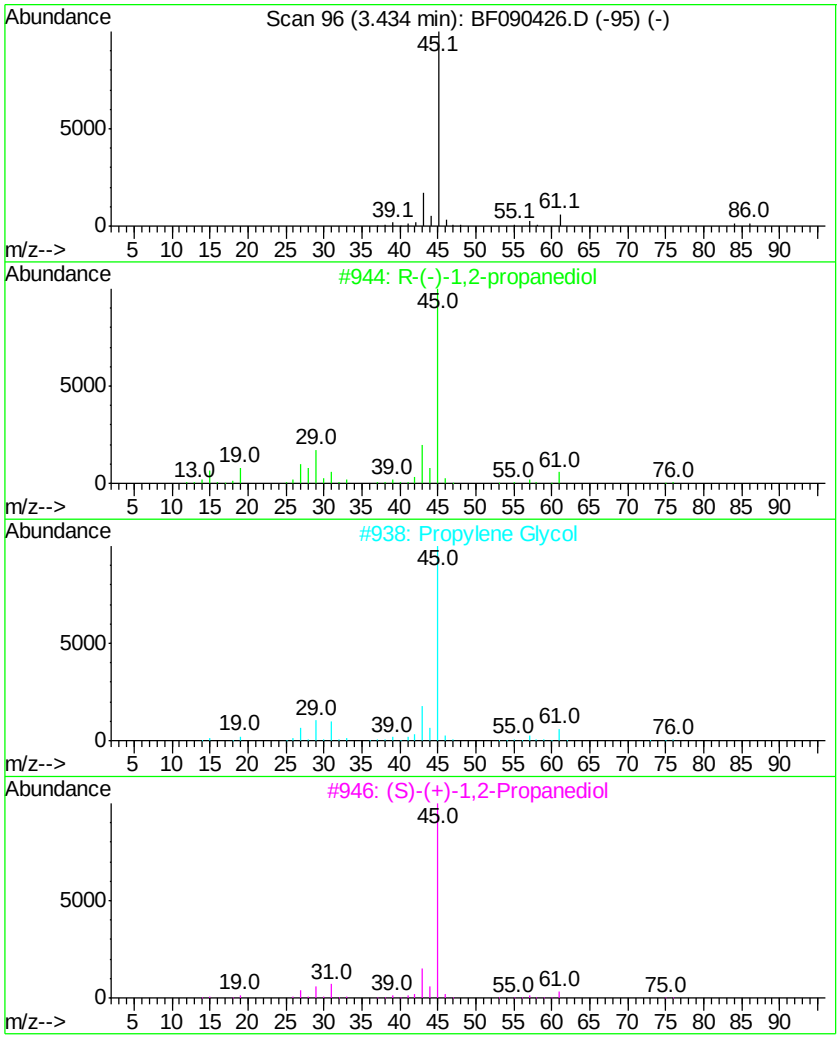
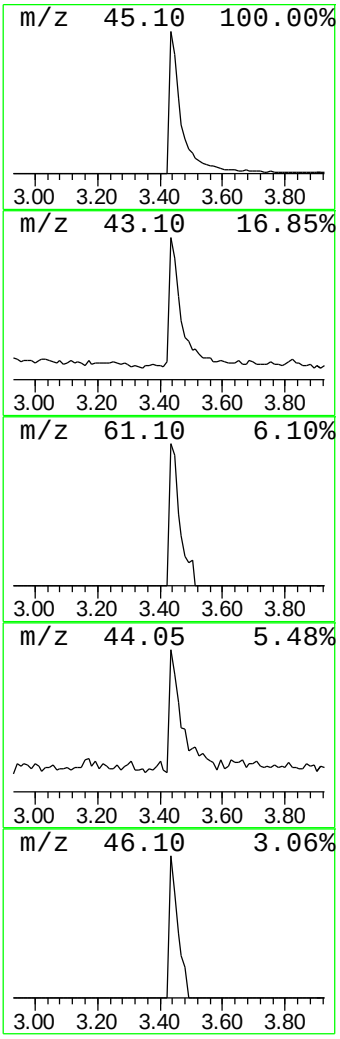
Peak Number 1 unknown3.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.43	2.65 ng	170857	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
5	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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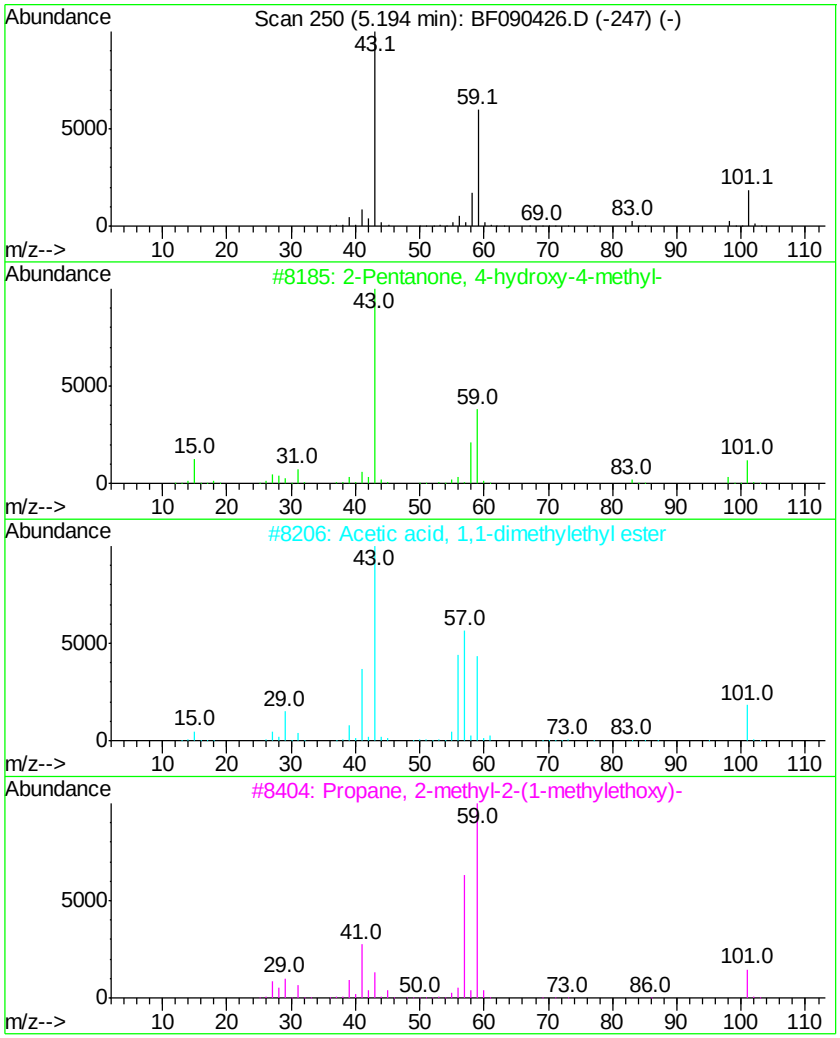
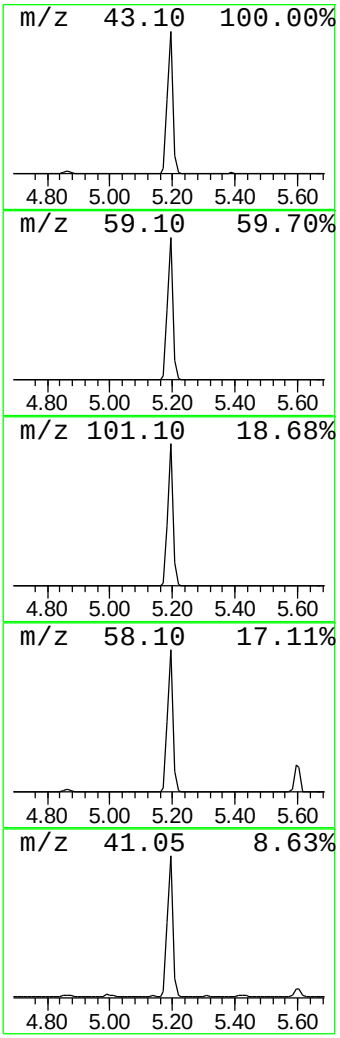
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	26.08 ng	1678250	1,4-Dichlorobenzene-d4	6.99

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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

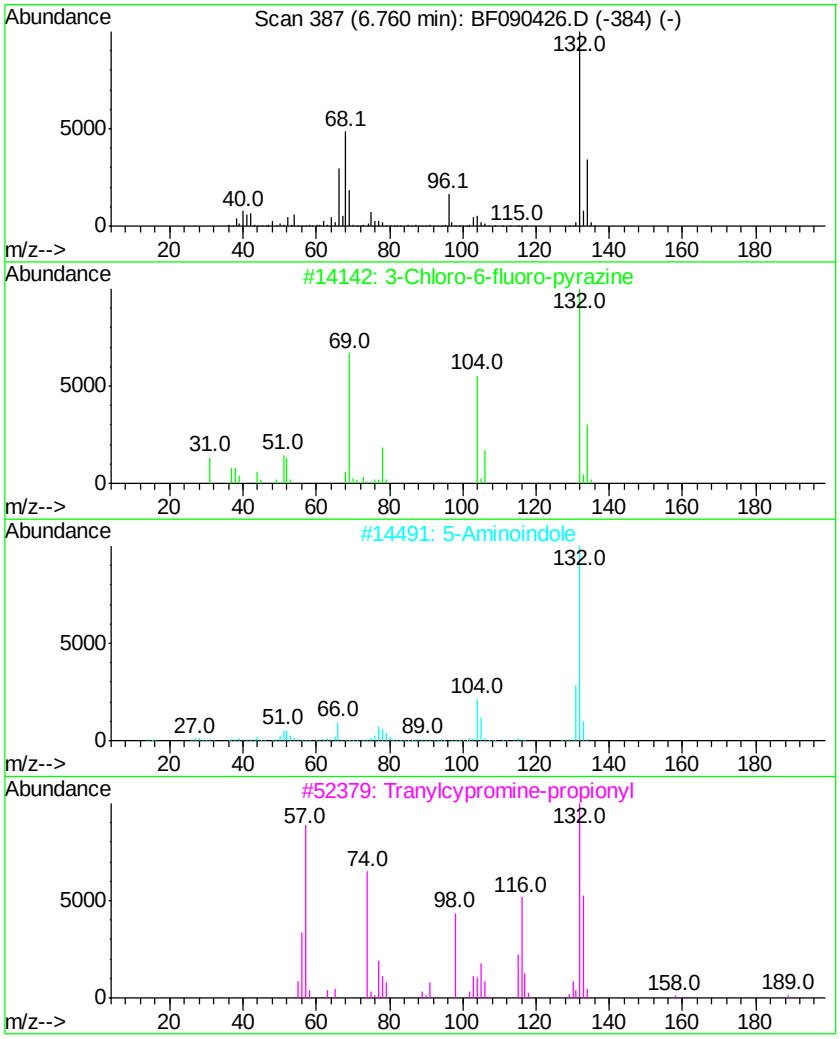
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

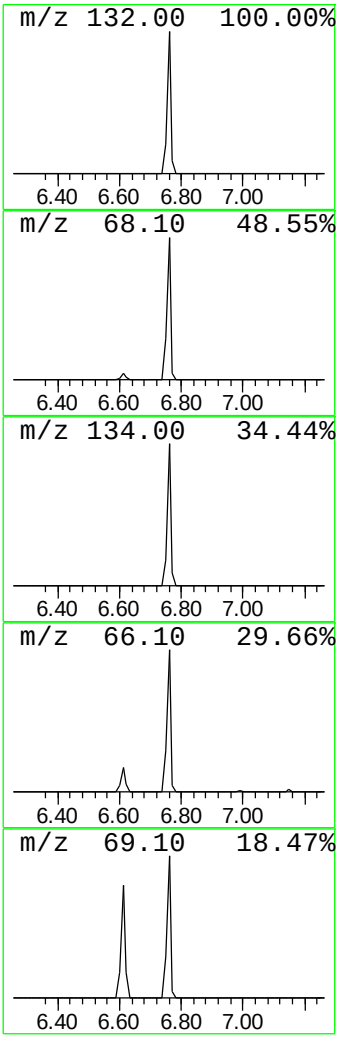
****

Peak Number 3 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	72.40 ng	4659140	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

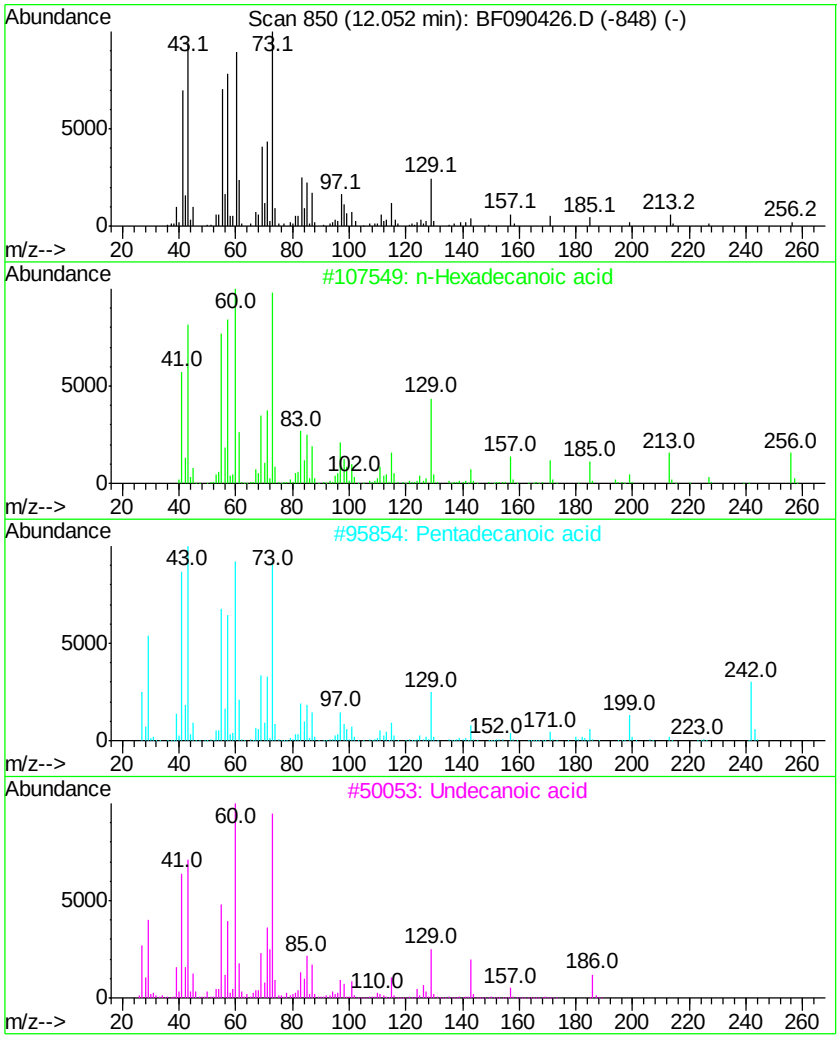
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

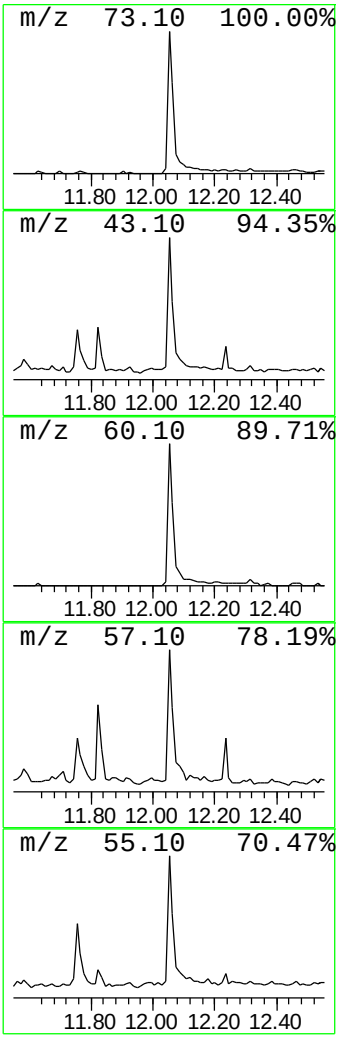
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	3.23 ng	342173	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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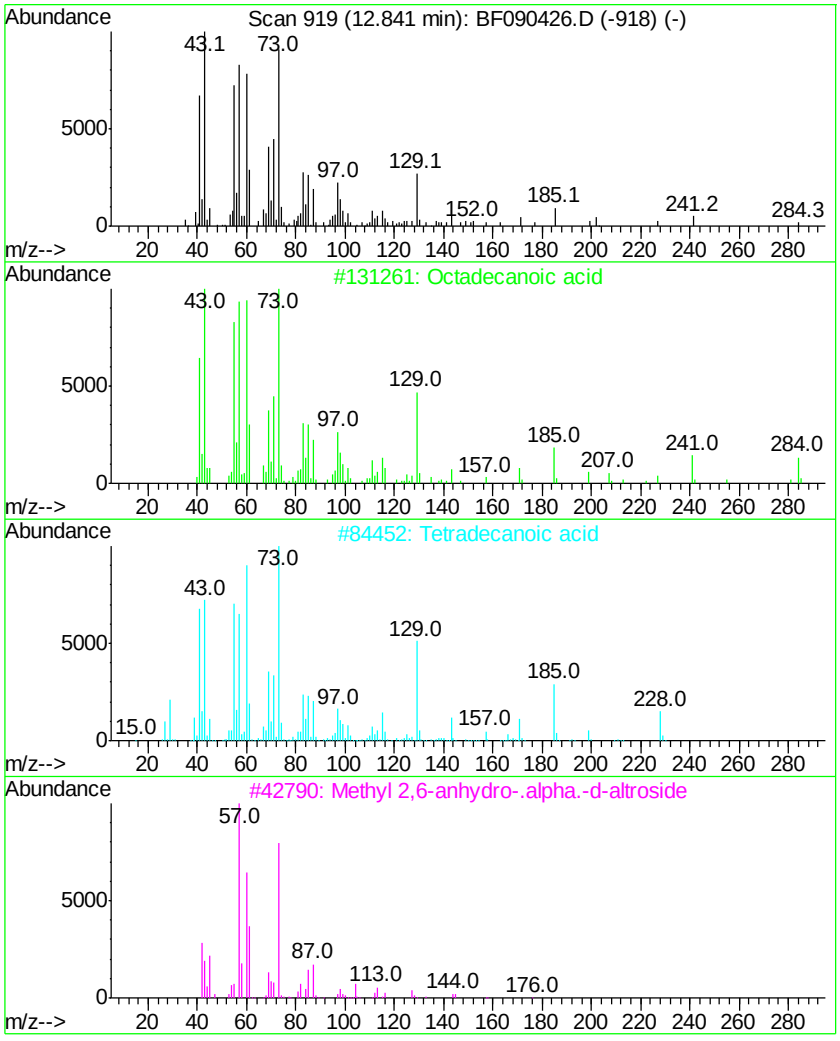
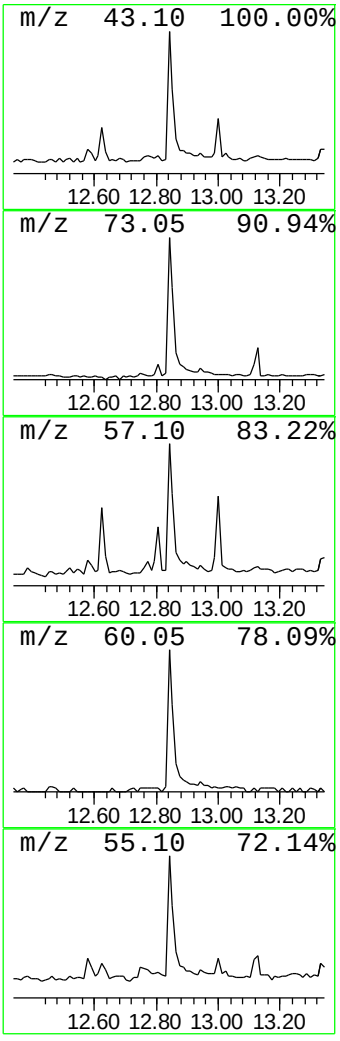
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.50 ng	264303	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	27
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

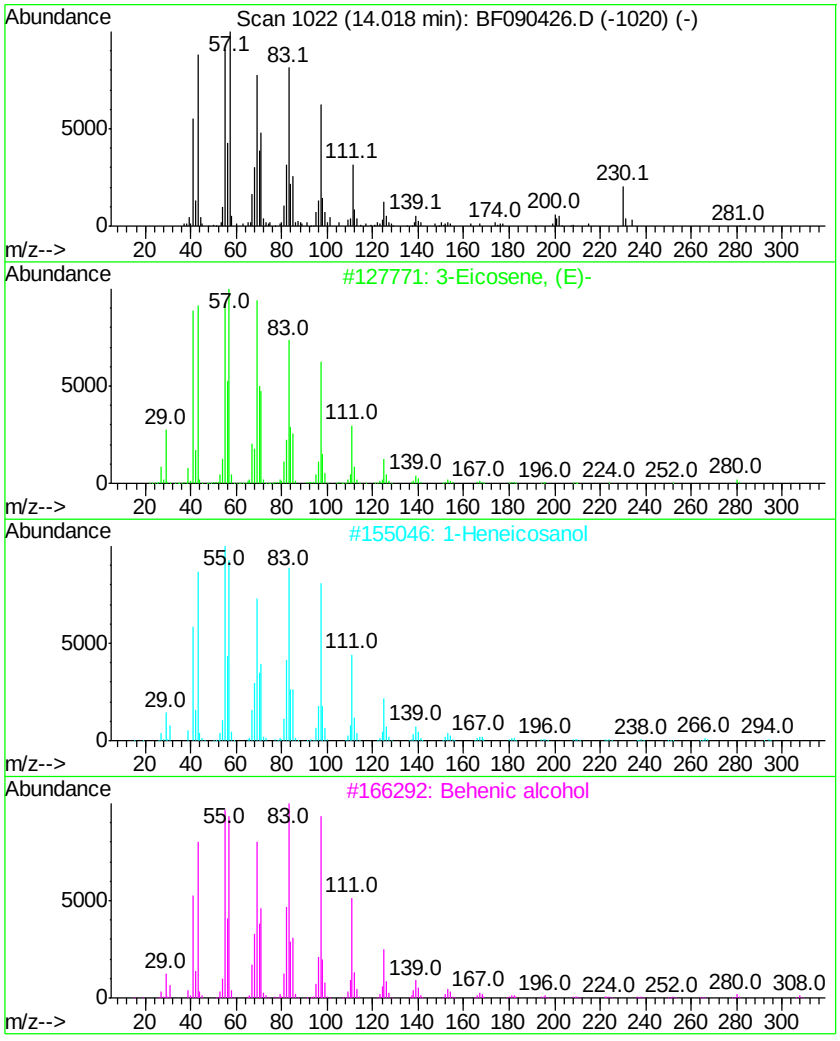
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

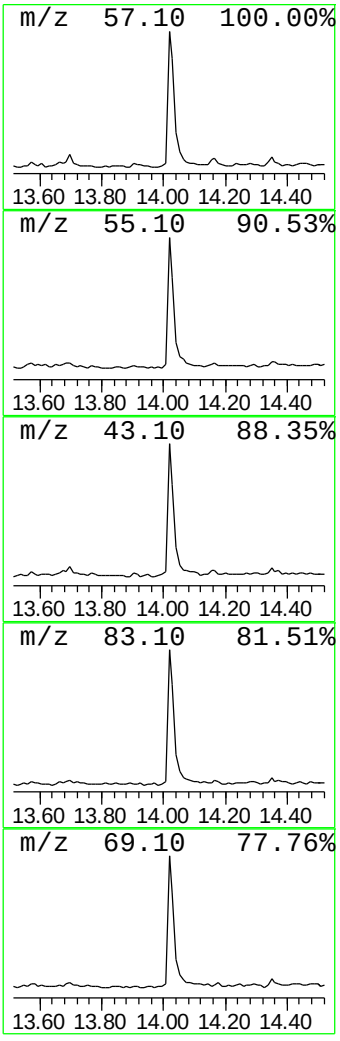
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	3.53 ng	375265	Chrysene-d12	14.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

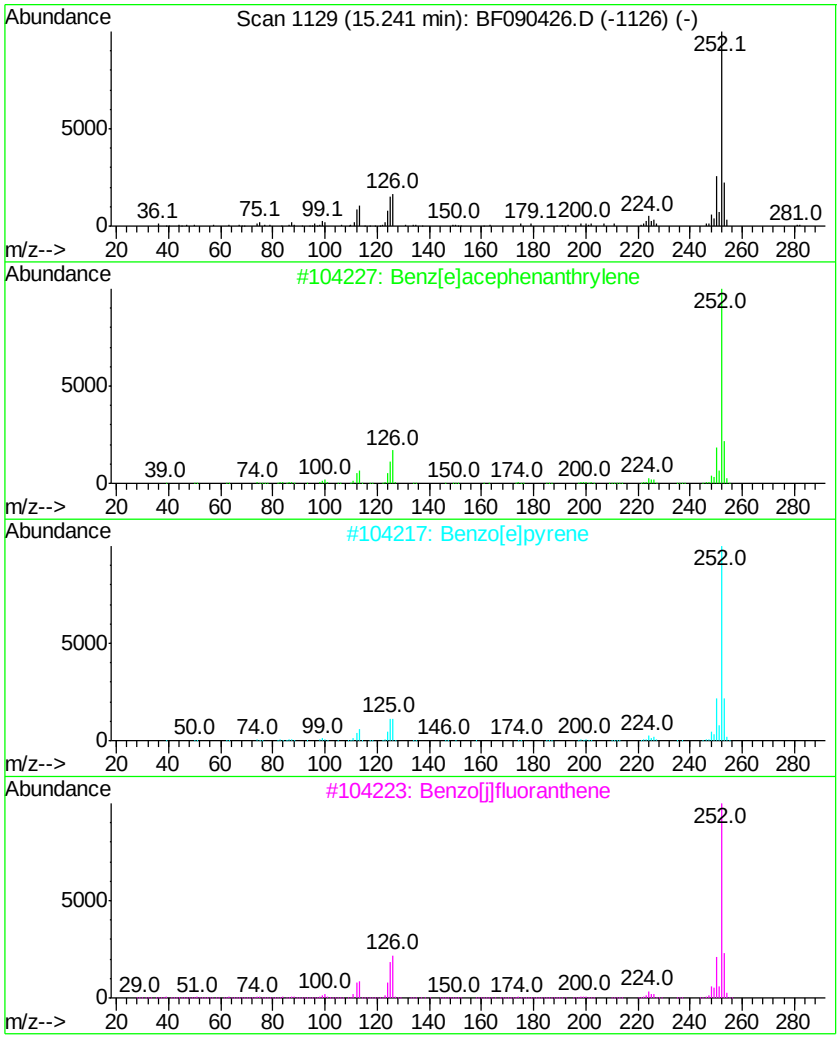
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

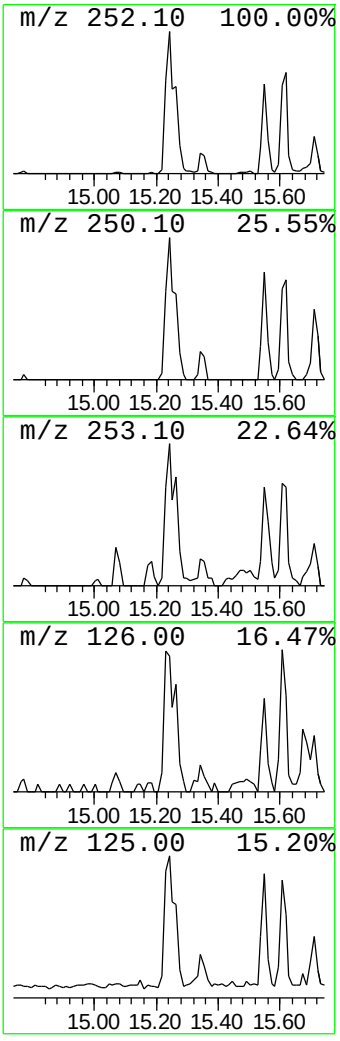
****

Peak Number 8 Benz[e]acephenanthrylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	3.37 ng	223433	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
4	Perylene	252	C20H12	000198-55-0	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100616\
Data File : BF090426.D
Acq On : 6 Oct 2016 18:58
Operator : UM/SJ
Sample : H5068-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S36-9003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
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
unknown3.43	3.43	2.6	ng	170857	1	6.99	1287090	20.0
2-Pentanone, 4-hy...	5.19	26.1	ng	1678250	1	6.99	1287090	20.0
unknown6.76	6.76	72.4	ng	4659140	1	6.99	1287090	20.0
n-Hexadecanoic acid	12.05	3.2	ng	342173	4	11.54	2117030	20.0
Octadecanoic acid	12.84	2.5	ng	264303	4	11.54	2117030	20.0
3-Eicosene, (E)-	14.02	3.5	ng	375265	5	14.18	2126600	20.0
Benz[e]acephenant...	15.24	3.4	ng	223433	6	15.69	1324060	20.0