LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

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-BF102116.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	5.046	235	237	246	rBV	443324	556960	7.60%	1.058%
2	5.468	271	274	276	rBV	3172828	3558461	48.58%	6.758%
3	6.486	361	363	372	rBV	1879606	2233272	30.49%	4.242%
4	6.623	372	375	378	rBV	4967881	5410160	73.87%	10.275%
5	6.851	393	395	400	rBV	1404843	1534875	20.96%	2.915%
6	7.011	406	409	411	rBV	5174068	5059547	69.08%	9.609%
7	7.423	442	445	447	rBV	3662336	4237523	57.86%	8.048%
8	7.880	483	485	487	rVV	112292	112353	1.53%	0.213%
9	8.143	505	508	516	rBV2	1990885	2644227	36.10%	5.022%
10	8.646	550	552	555	rVB	209608	221626	3.03%	0.421%
11	8.703	555	557	561	rBV4	47560	93238	1.27%	0.177%
12	8.955	575	579	580	rBV2	81486	149565	2.04%	0.284%
13	9.217	599	602	605	rBV	5908718	7324343	100.00%	13.911%
14	9.560	630	632	635	rBV4	33881	88052	1.20%	0.167%
15	9.617	635	637	639	rVB	301946	413946	5.65%	0.786%
16	9.892	659	661	663	rBV	2211249	2184909	29.83%	4.150%
17	9.926	663	664	666	rVB	768666	574795	7.85%	1.092%
18	10.098	677	679	686	rBV	149375	227481	3.11%	0.432%
19	10.692	727	731	733	rBV	3264123	4403868	60.13%	8.364%
20	10.806	739	741	745	rVB	147790	211370	2.89%	0.401%
21	11.378	789	791	795	rBV	1934900	1927486	26.32%	3.661%
22	11.926	837	839	843	rBV2	184251	242536	3.31%	0.461%
23	11.995	843	845	848	rVB	72677	79262	1.08%	0.151%
24	12.589	895	897	900	rVB	219250	180145	2.46%	0.342%
25	12.704	905	907	909	rBV	143520	170947	2.33%	0.325%
26	12.818	915	917	919	rBV	120223	118325	1.62%	0.225%
27	12.966	928	930	933	rBV	4294161	5415522	73.94%	10.285%
28	13.869	1007	1009	1012	rBV	140049	168267	2.30%	0.320%
29	14.018	1020	1022	1029	rBV	1276328	1254641	17.13%	2.383%
30	15.458	1145	1148	1165	rVB	887936	1433354	19.57%	2.722%
31	15.904	1185	1187	1190	rVB	50985	73642	1.01%	0.140%
32	16.384	1227	1229	1236	rVB2	68589	156994	2.14%	0.298%
33	16.955	1276	1279	1283	rVB	39194	84996	1.16%	0.161%
34	17.630	1334	1338	1343	rVB	37085	105685	1.44%	0.201%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103S

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-BF102116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

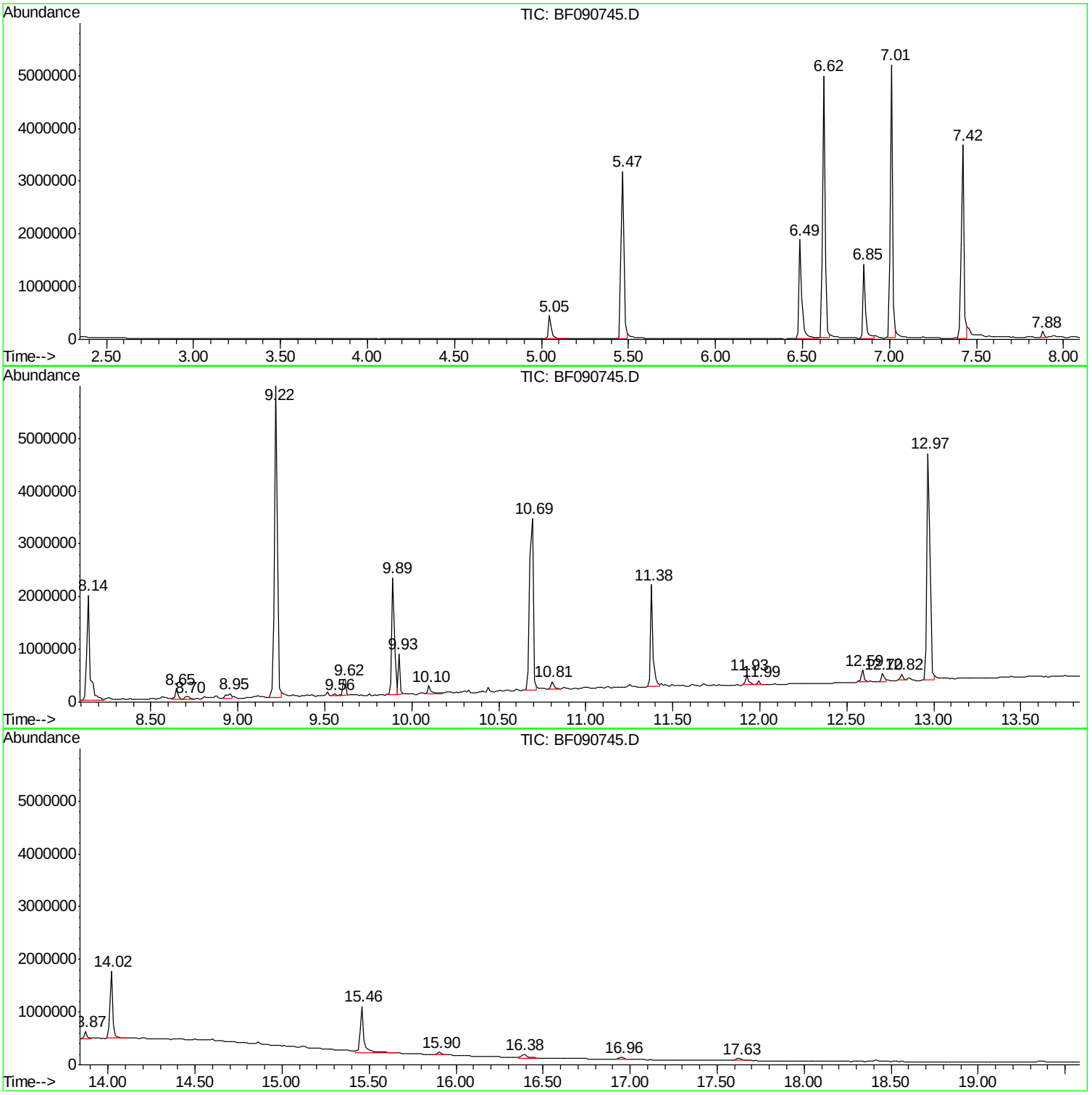
Sum of corrected areas: 52652373

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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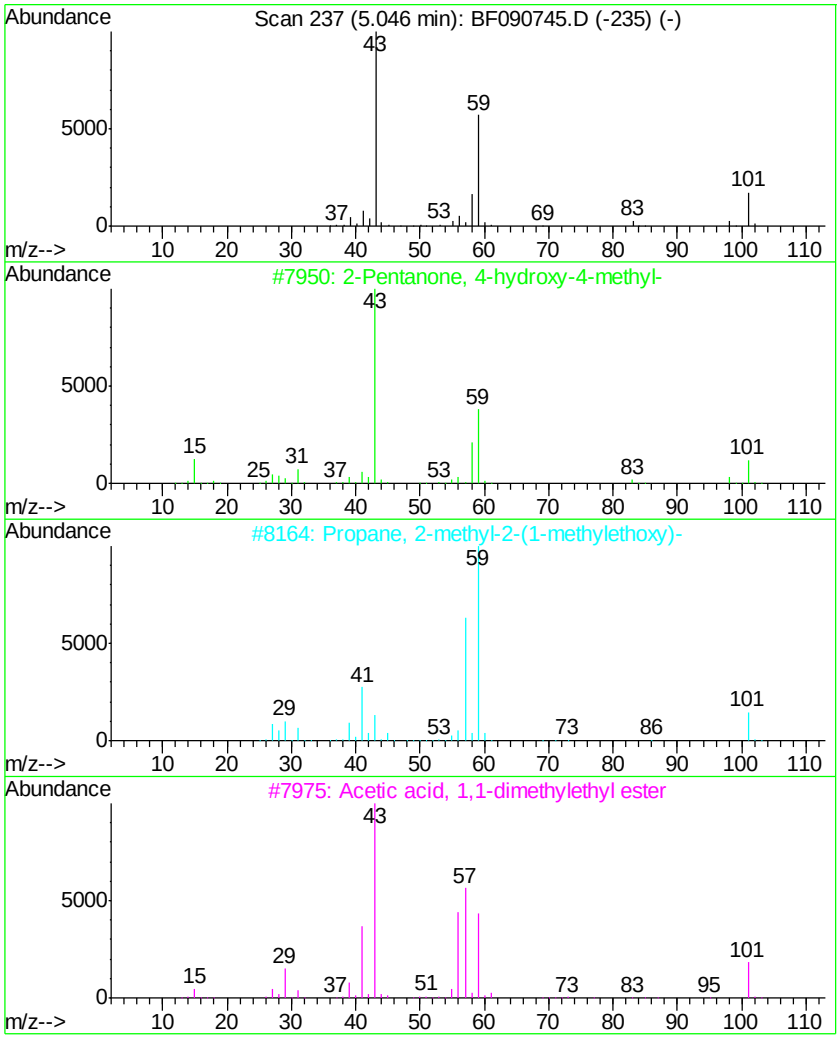
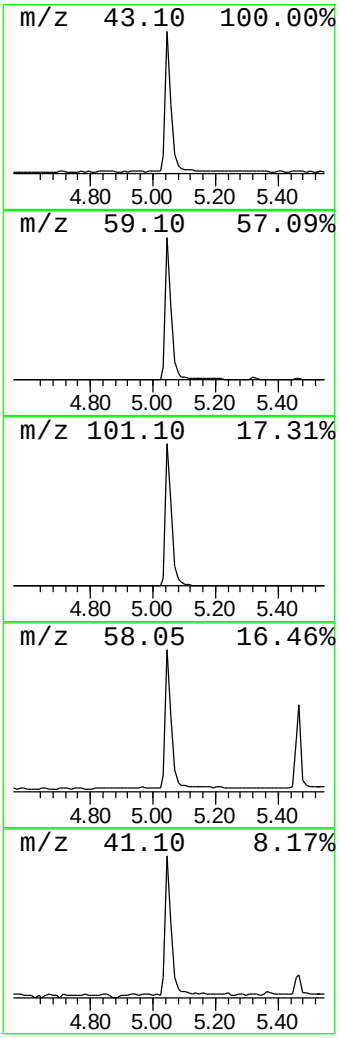
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	7.26 ng	556960	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

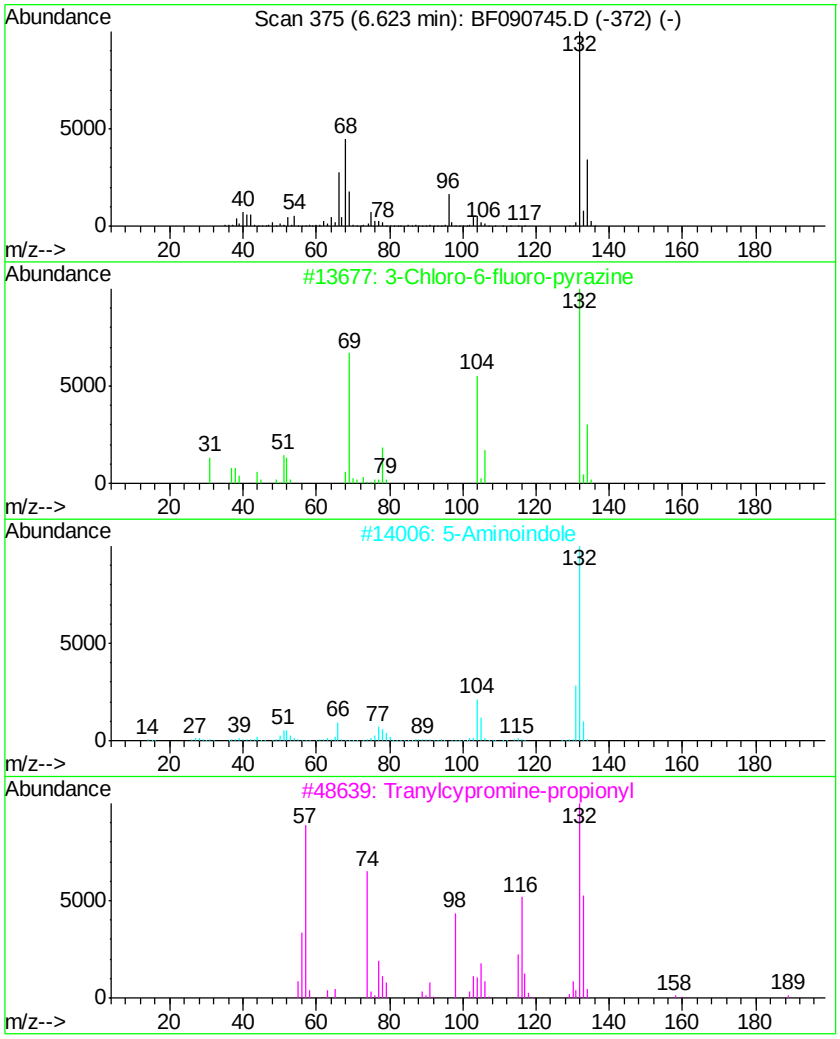
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

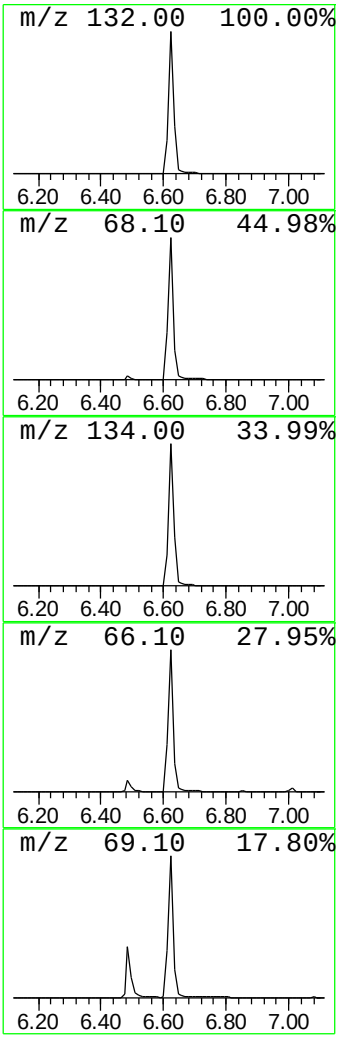
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.50 ng	5410160	1,4-Dichlorobenzene-d4	6.85

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

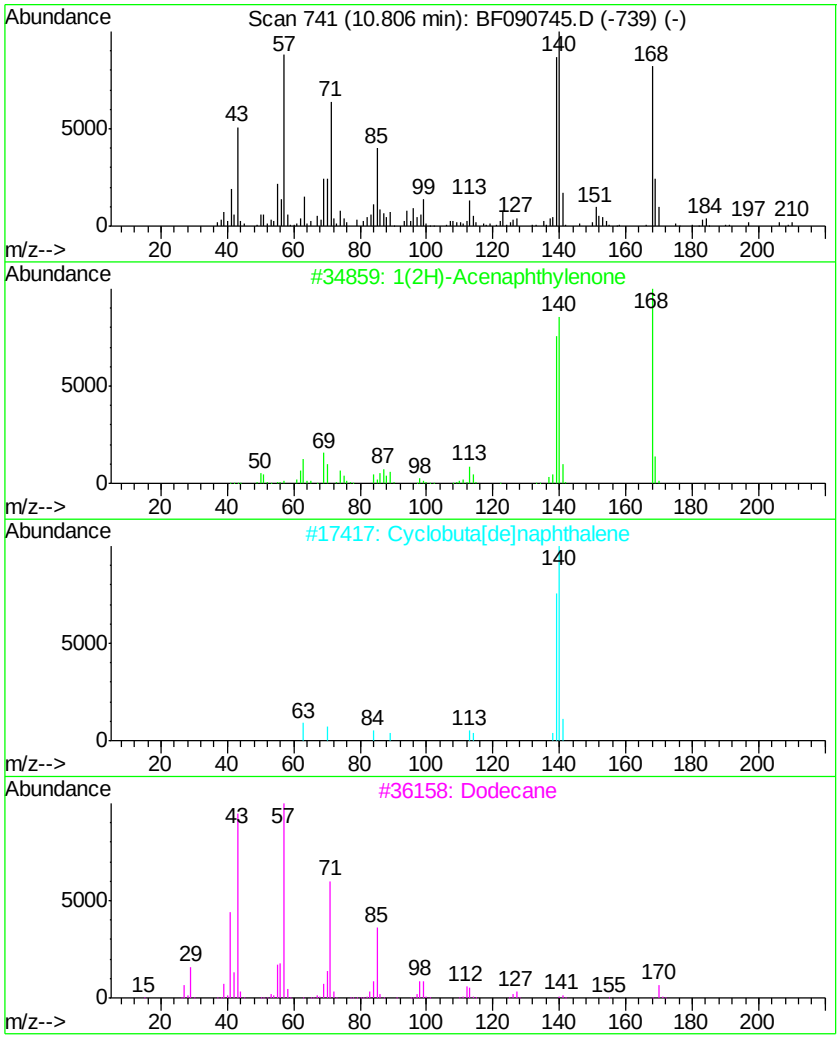
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

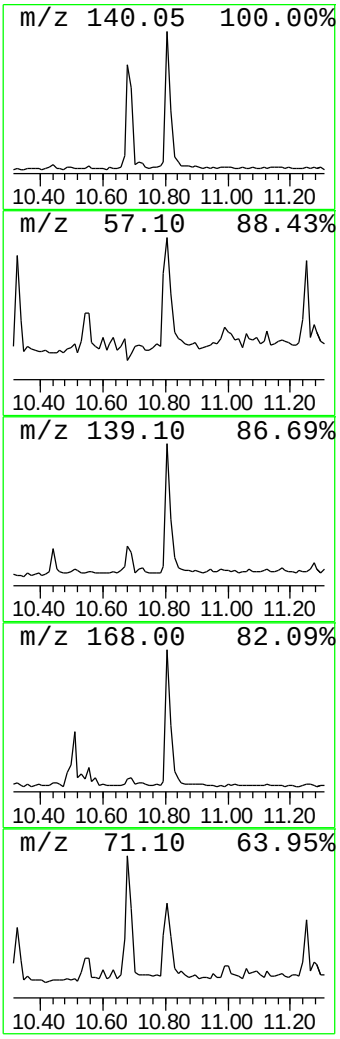
****

Peak Number 5 1(2H)-Acenaphthylenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.19 ng	211370	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	93
2	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	38
3	Dodecane	170	C12H26	000112-40-3	25
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	18
5	Tridecane	184	C13H28	000629-50-5	11





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

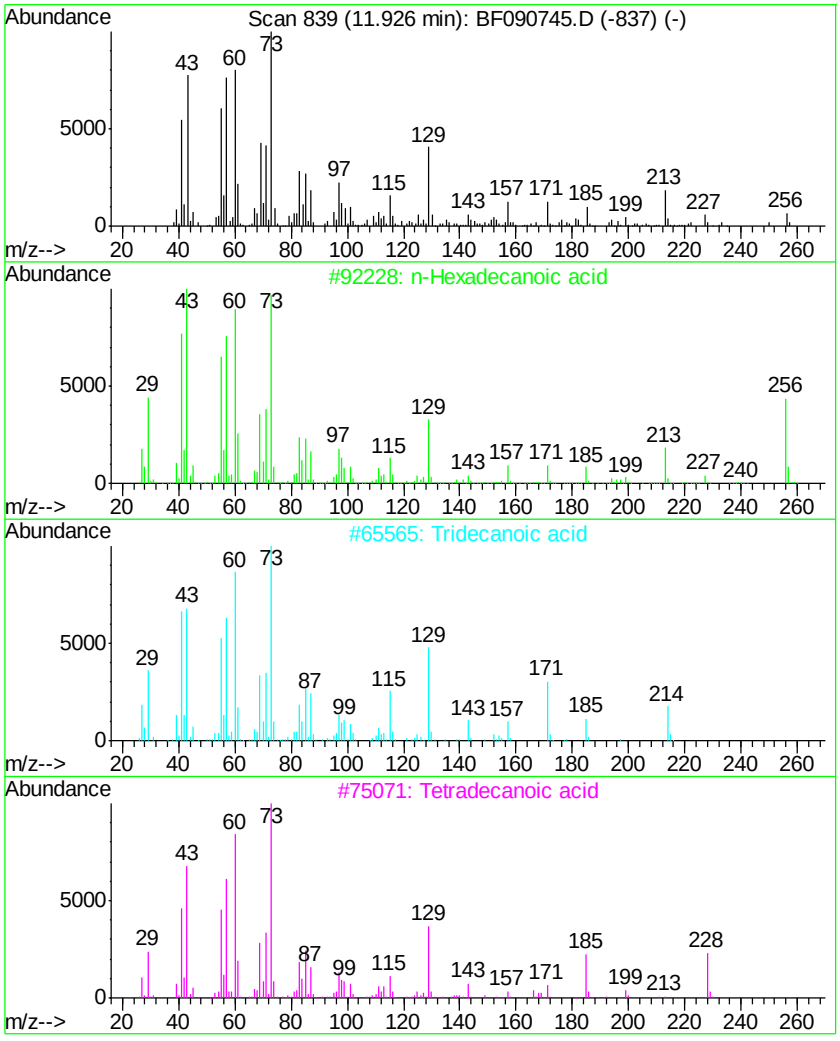
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

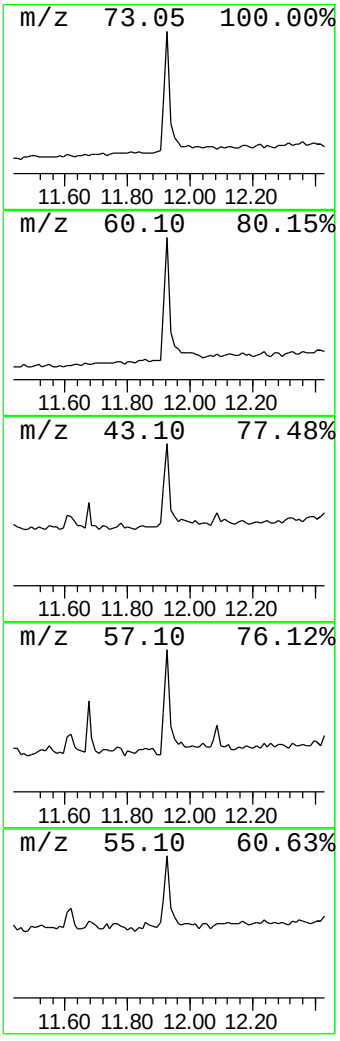
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.52 ng	242536	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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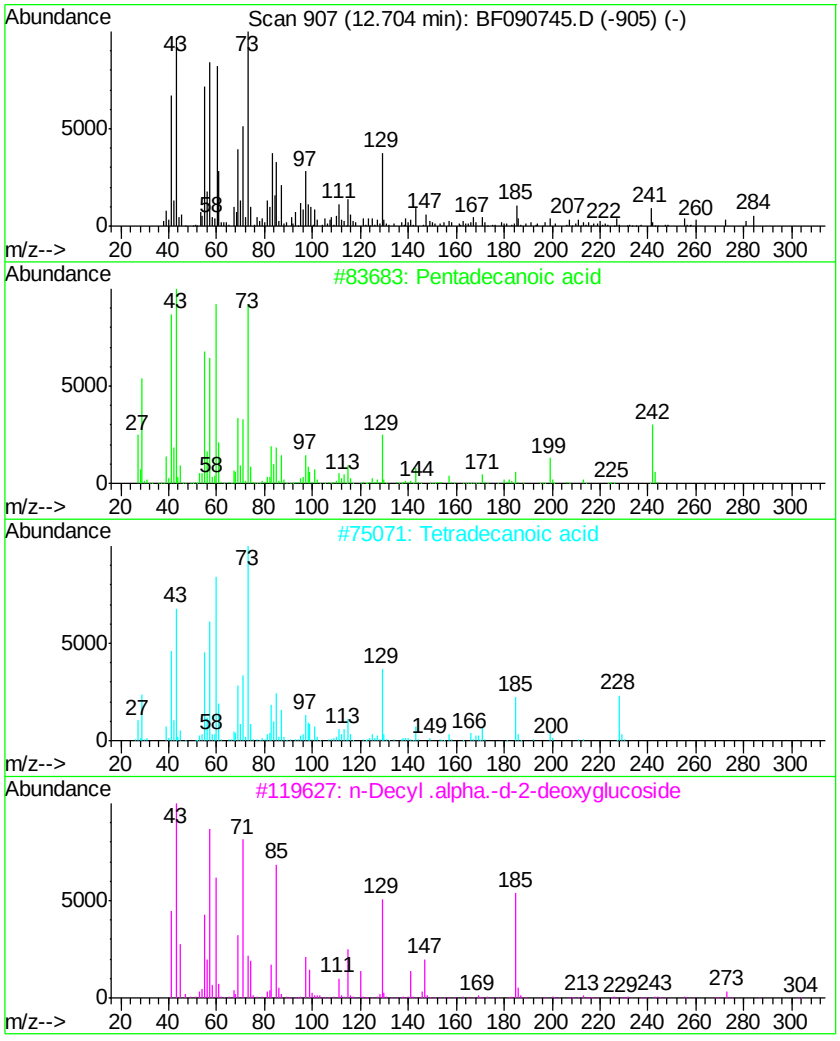
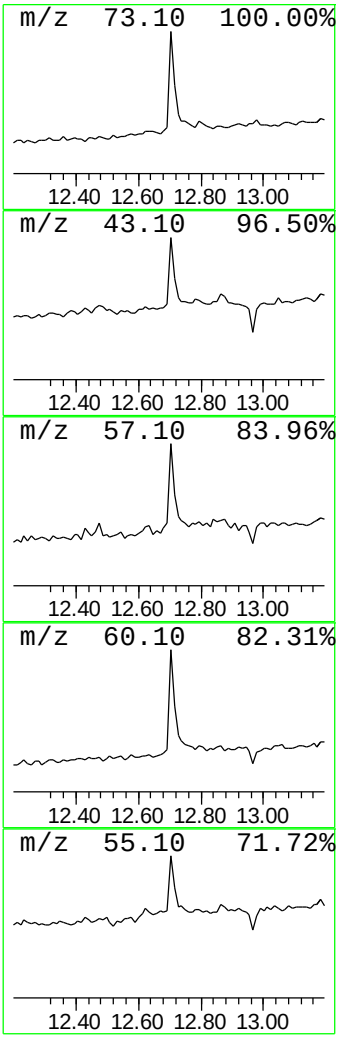
Peak Number 7 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.73 ng	170947	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	27
4	Hexadecane	226	C16H34	000544-76-3	25
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	15





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Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

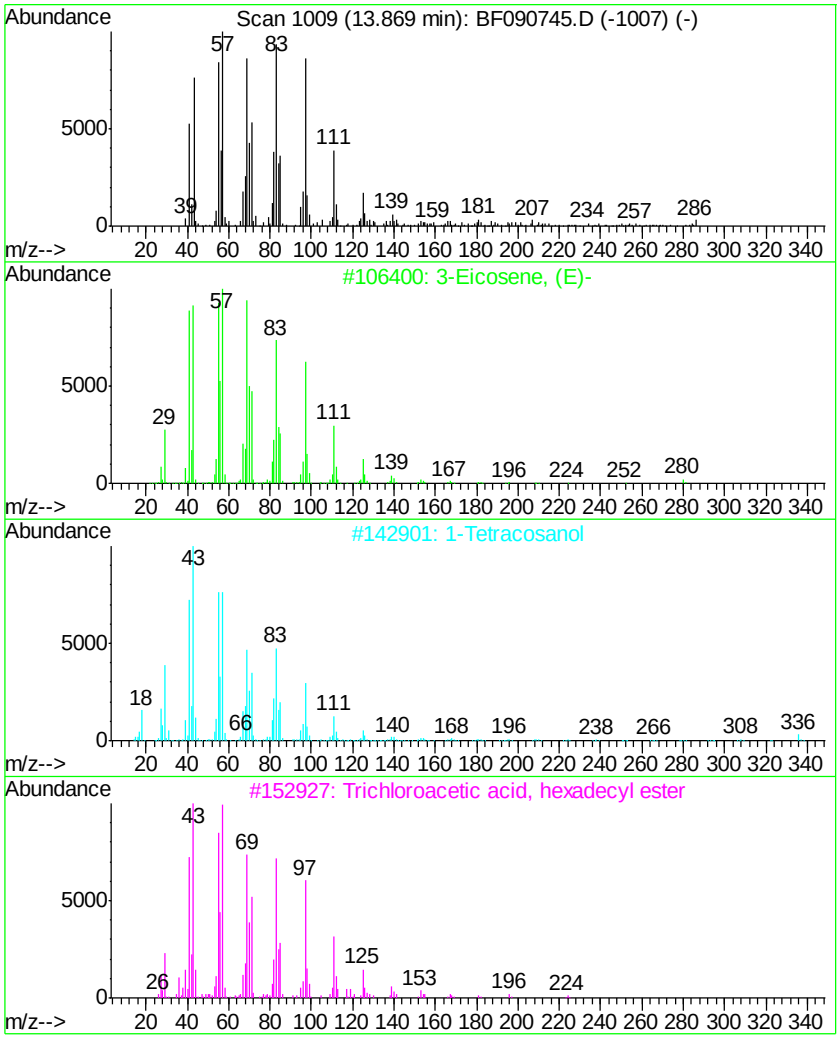
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

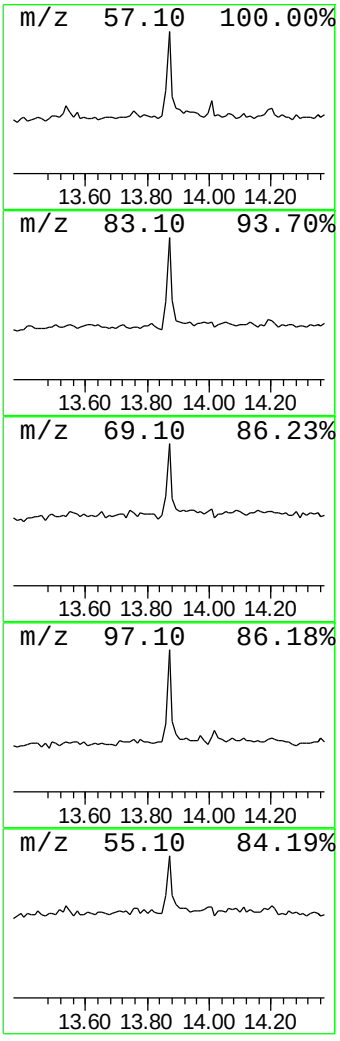
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.68 ng	168267	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Tetracosanol	354	C24H50O	000506-51-4	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	1-Pentadecanol	228	C15H32O	000629-76-5	83
5	1-Heptadecanol	256	C17H36O	001454-85-9	83





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Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

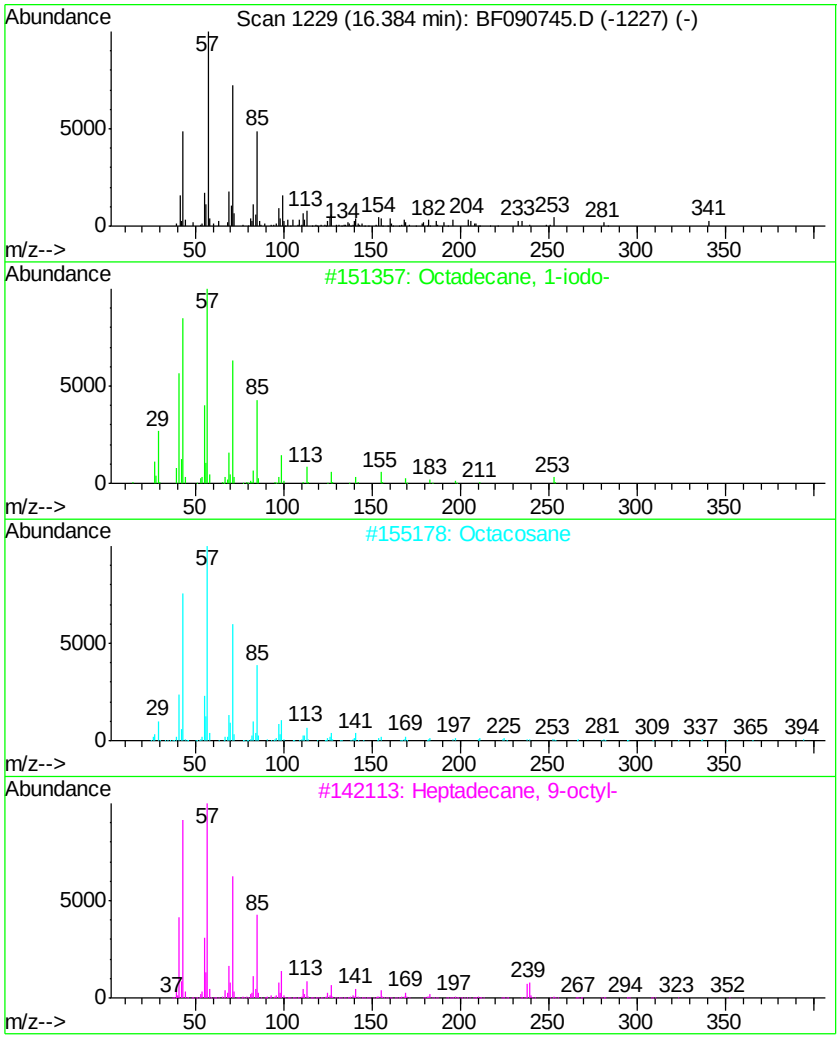
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

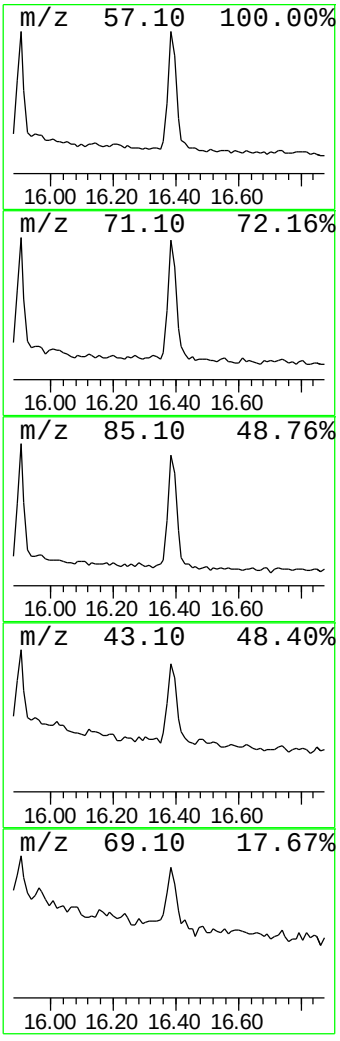
****

Peak Number 9 Octadecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	2.19 ng	156994	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
2	Octacosane	394	C28H58	000630-02-4	83
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Nonadecane	268	C19H40	000629-92-5	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102116\
Data File : BF090745.D
Acq On : 22 Oct 2016 7:24
Operator : UM/SJ
Sample : H5308-20
Misc :
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Instrument : BNA_F
ClientSampleId : MW-103S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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	7.3	ng	556960	1	6.85	1534880	20.0
unknown6.62	6.62	70.5	ng	5410160	1	6.85	1534880	20.0
1(2H)-Acenaphthyl...	10.81	2.2	ng	211370	4	11.38	1927490	20.0
n-Hexadecanoic acid	11.93	2.5	ng	242536	4	11.38	1927490	20.0
Pentadecanoic acid	12.70	2.7	ng	170947	5	14.02	1254640	20.0
3-Eicosene, (E)-	13.87	2.7	ng	168267	5	14.02	1254640	20.0
Octadecane, 1-iodo-	16.38	2.2	ng	156994	6	15.46	1433350	20.0