LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
Data File : BF090399.D
Acq On : 6 Oct 2016 00:12
Operator : UM/SJ
Sample : H5061-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

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	3.457	95	98	114	rBV	121220	286929	4.61%	0.521%
2	5.206	248	251	254	rBV	1114844	1373127	22.07%	2.495%
3	5.606	283	286	289	rBV	4522225	5622859	90.39%	10.218%
4	6.623	372	375	377	rBV	5716567	5839702	93.87%	10.612%
5	6.772	385	388	390	rBV	5889621	6220801	100.00%	11.305%
6	7.000	406	408	410	rBV	1783526	1439161	23.13%	2.615%
7	7.160	419	422	424	rVB	4761802	4227131	67.95%	7.682%
8	7.560	454	457	460	rBV	3608499	3433307	55.19%	6.239%
9	7.640	460	464	466	rVB	87868	104552	1.68%	0.190%
10	8.292	518	521	523	rBV	1999587	1950184	31.35%	3.544%
11	9.366	612	615	618	rBV	5732840	5211349	83.77%	9.470%
12	9.766	647	650	651	rBV	1494967	1820611	29.27%	3.308%
13	10.052	672	675	677	rVB	2465499	2158826	34.70%	3.923%
14	10.486	709	713	714	rBV	78933	107706	1.73%	0.196%
15	10.841	741	744	746	rBV	4025677	3820252	61.41%	6.942%
16	10.955	752	754	759	rVB	130536	145862	2.34%	0.265%
17	11.412	791	794	795	rBV	59234	83738	1.35%	0.152%
18	11.538	803	805	808	rBV	2209275	1902904	30.59%	3.458%
19	11.778	823	826	829	rBV	31335	64063	1.03%	0.116%
20	11.835	829	831	833	rVB	78585	64646	1.04%	0.117%
21	12.063	849	851	865	rVB	659485	726509	11.68%	1.320%
22	12.772	909	913	918	rBV2	46040	116106	1.87%	0.211%
23	12.852	918	920	927	rVV	403529	440526	7.08%	0.801%
24	13.138	942	945	947	rBV2	3470060	4699202	75.54%	8.539%
25	13.607	981	986	990	rBV2	32923	86345	1.39%	0.157%
26	14.041	1021	1024	1032	rBV	187214	378915	6.09%	0.689%
27	14.189	1034	1037	1039	rBV	1549773	1453519	23.37%	2.641%
28	15.058	1111	1113	1116	rBV	92161	124053	1.99%	0.225%
29	15.687	1165	1168	1171	rBV	755298	1059499	17.03%	1.925%
30	16.292	1217	1221	1226	rBV5	17030	66898	1.08%	0.122%

Sum of corrected areas: 55029282

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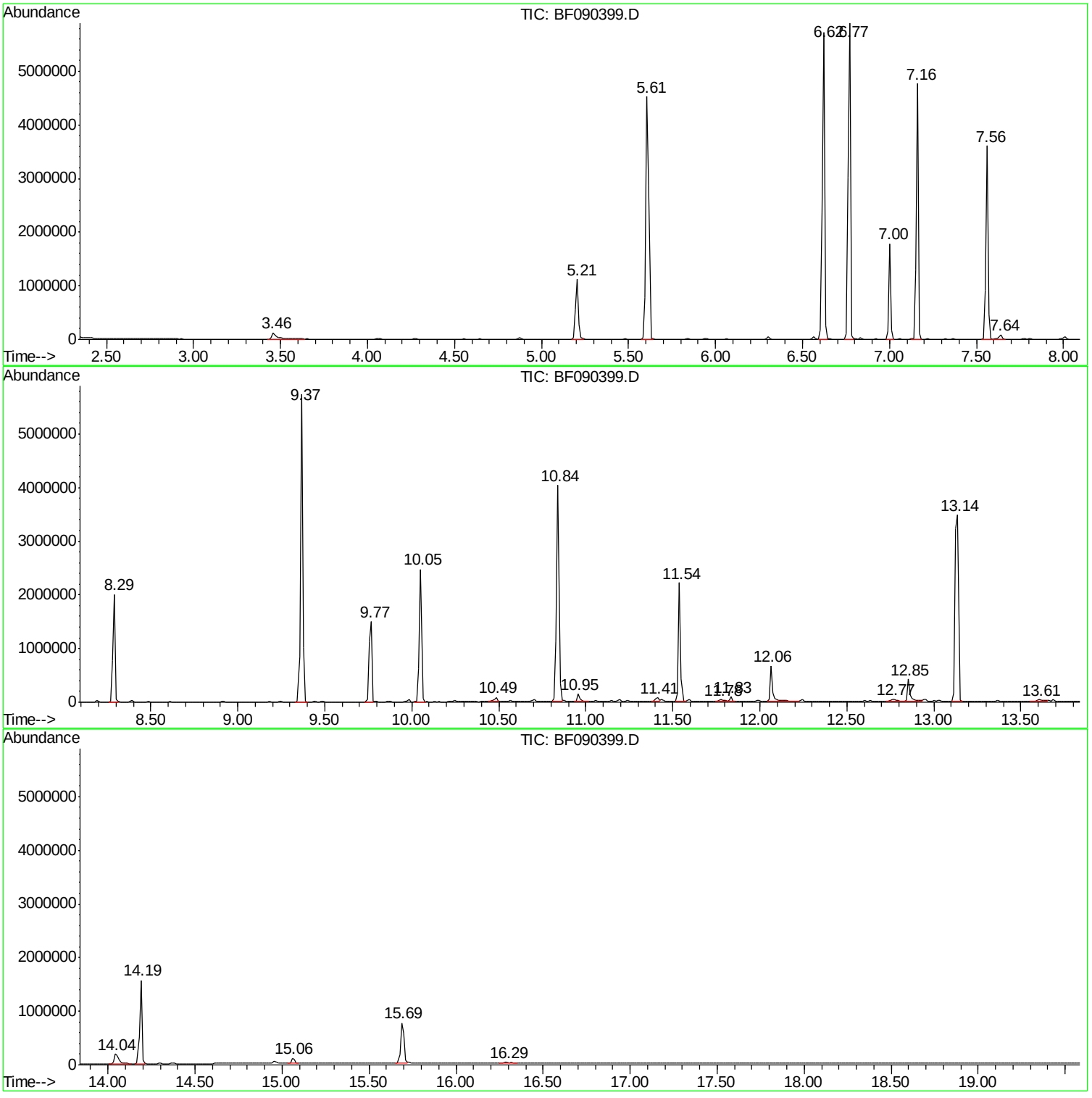
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B003-5-10

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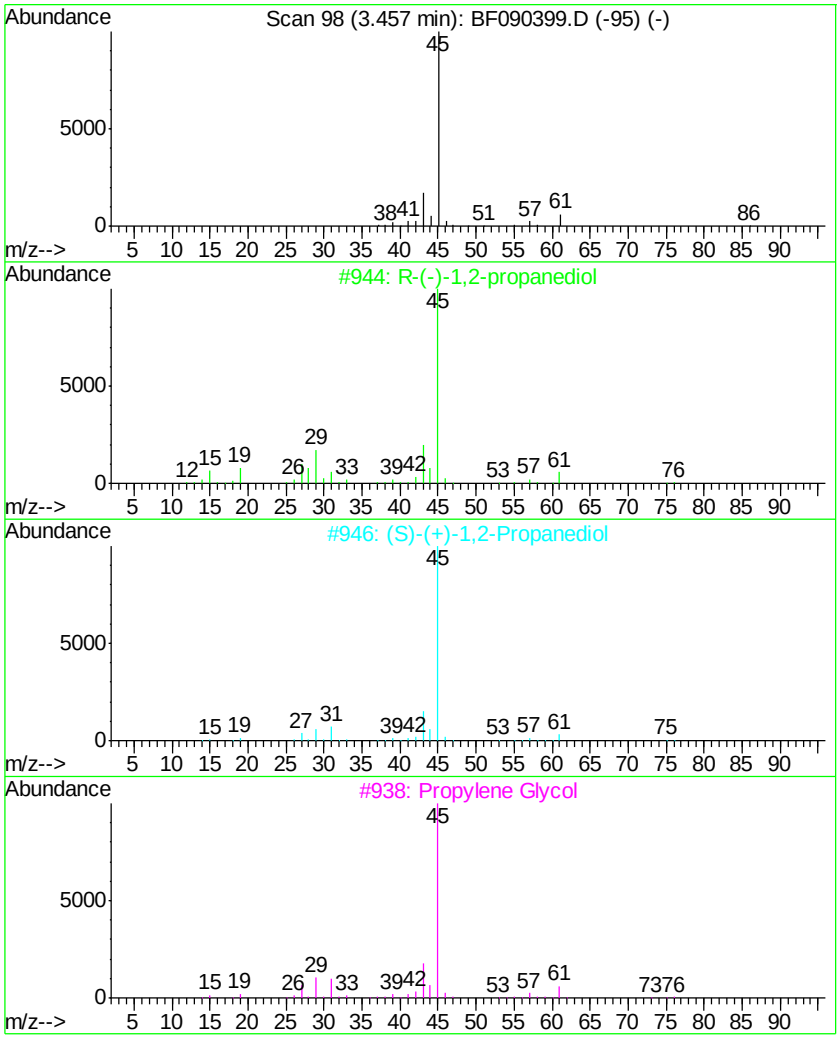
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

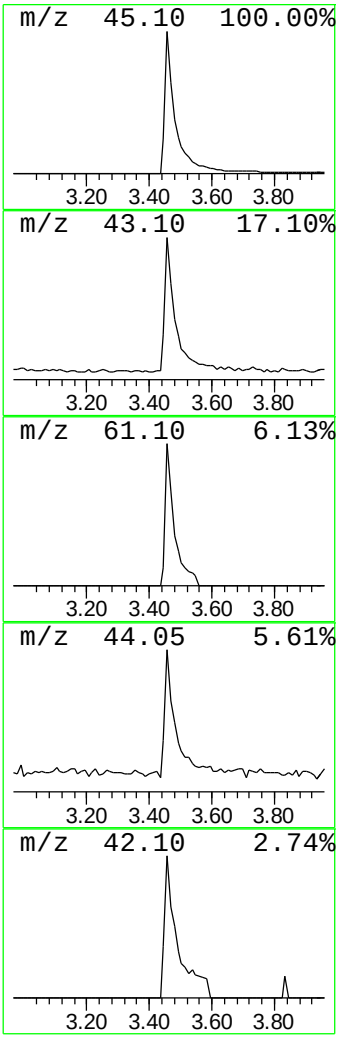
****

Peak Number 1 unknown3.46 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	3.99 ng	286929	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	Methyltartronic acid	134	C4H6O5	000595-98-2	9
5	2-Butanol	74	C4H10O	000078-92-2	9





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Data File : BF090399.D
Acq On : 6 Oct 2016 00:12
Operator : UM/SJ
Sample : H5061-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

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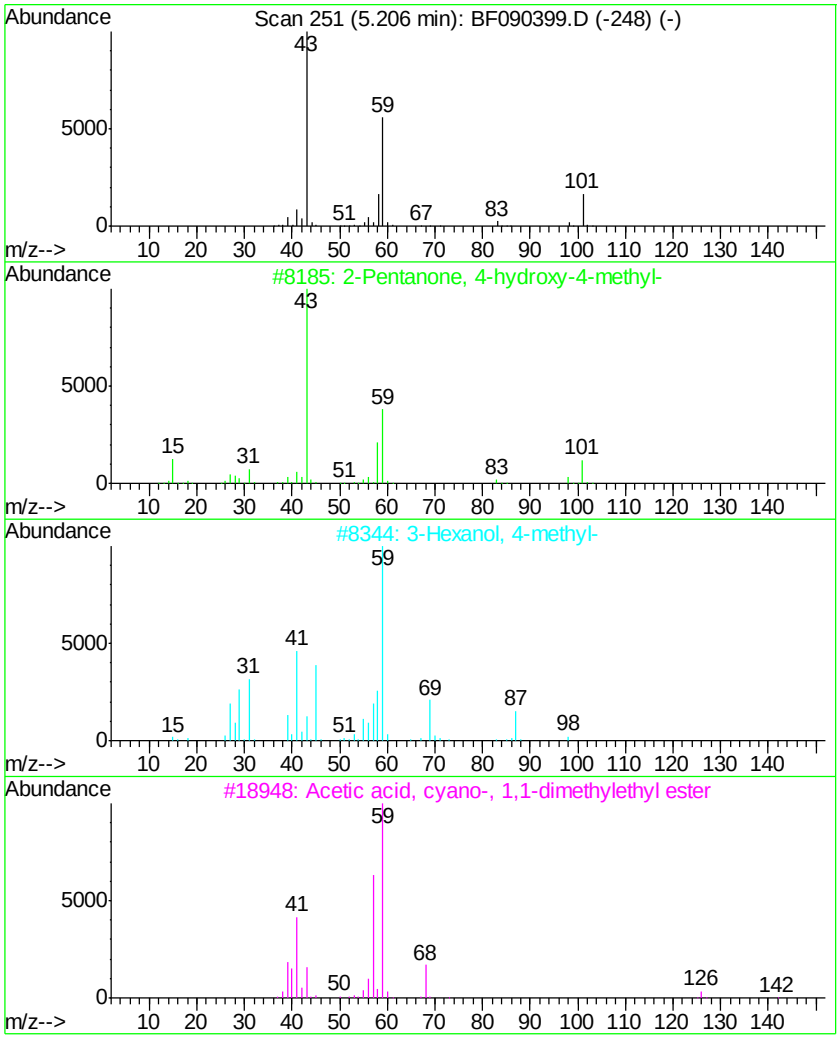
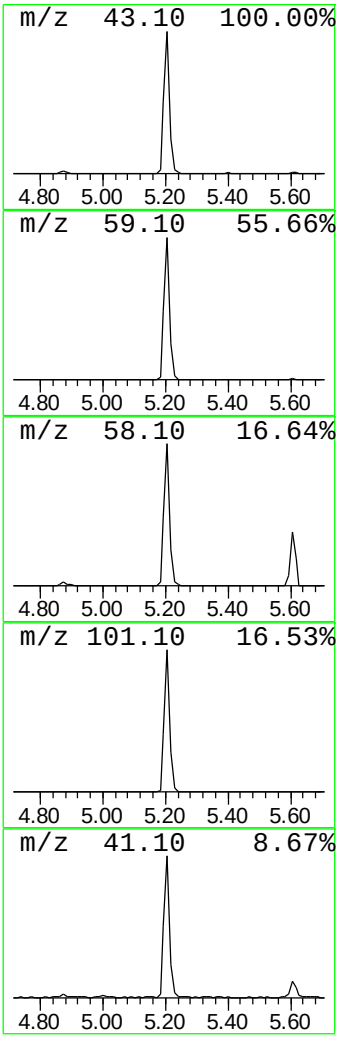
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	19.08 ng	1373130	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





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Sample : H5061-17
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Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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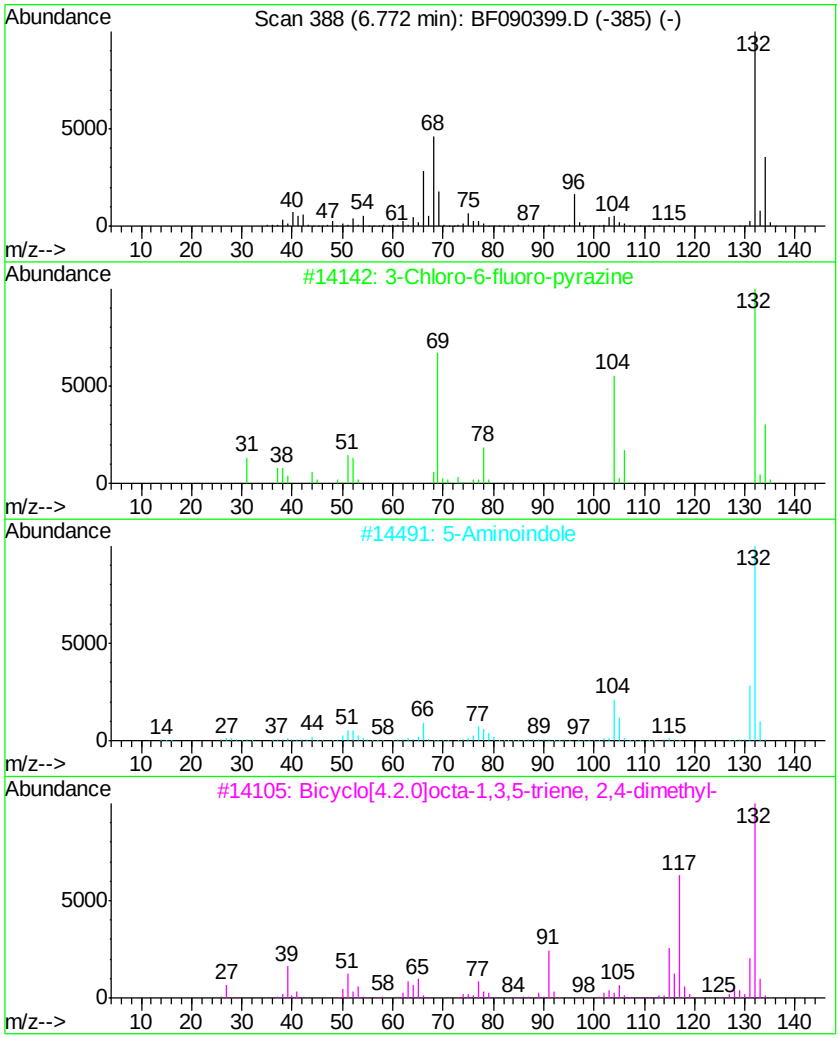
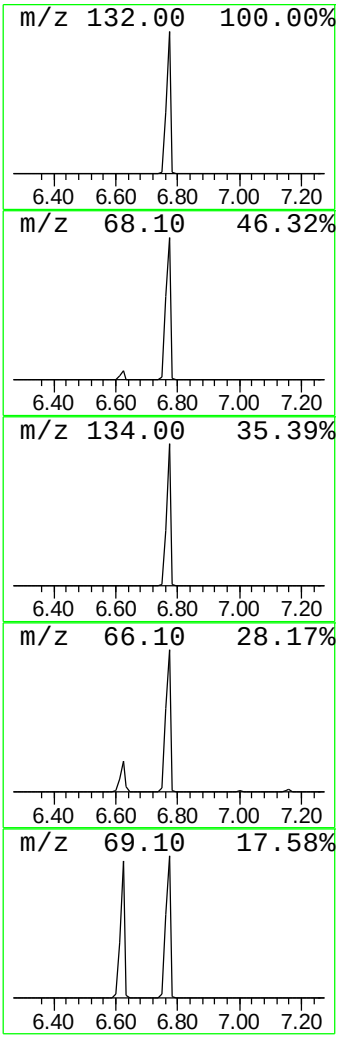
Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	86.45 ng	6220800	1,4-Dichlorobenzene-d4	7.00

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : H5061-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

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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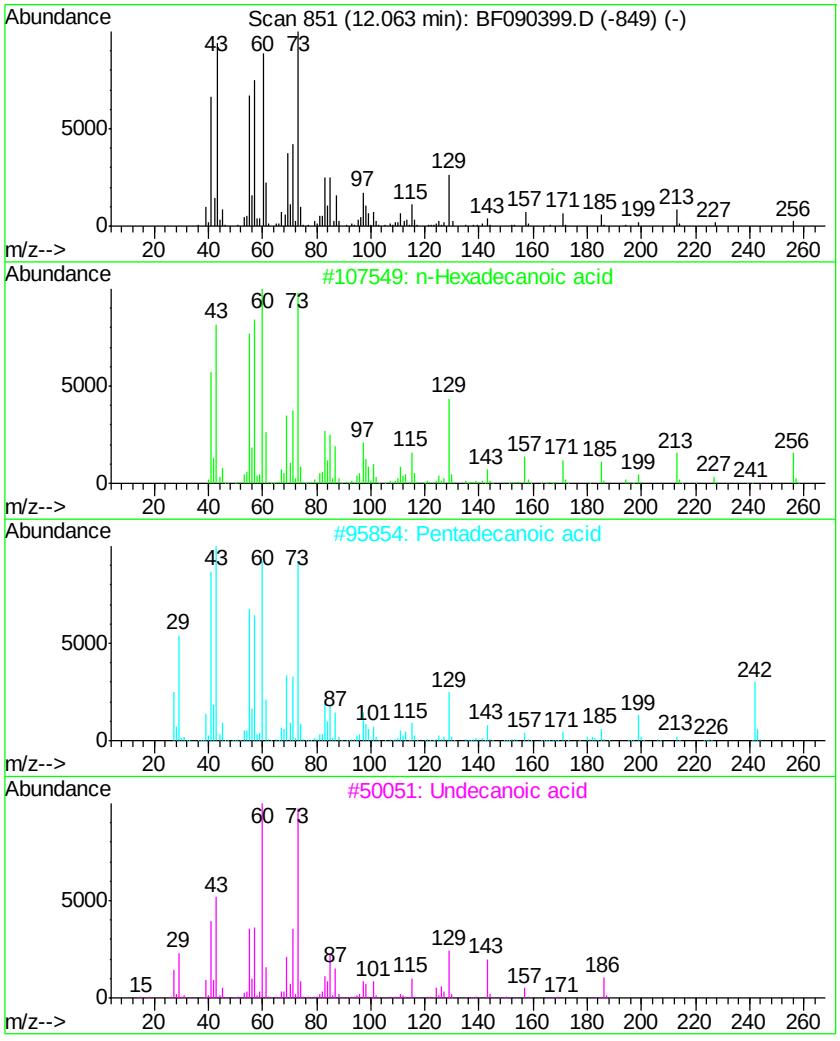
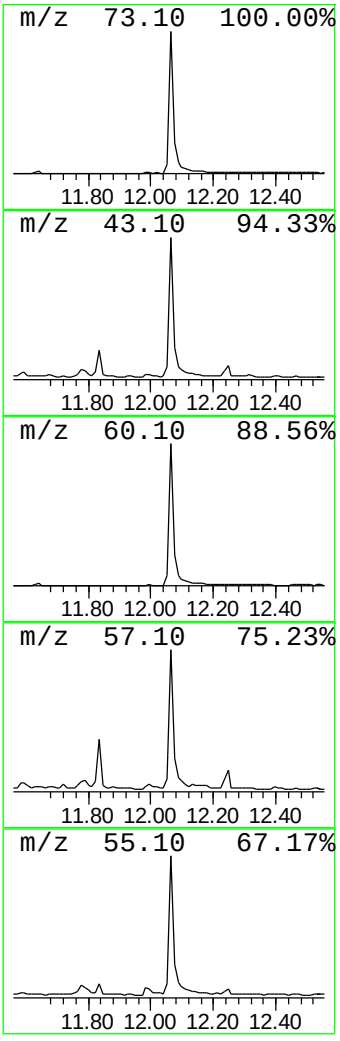
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	7.64 ng	726509	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100516\
Data File : BF090399.D
Acq On : 6 Oct 2016 00:12
Operator : UM/SJ
Sample : H5061-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

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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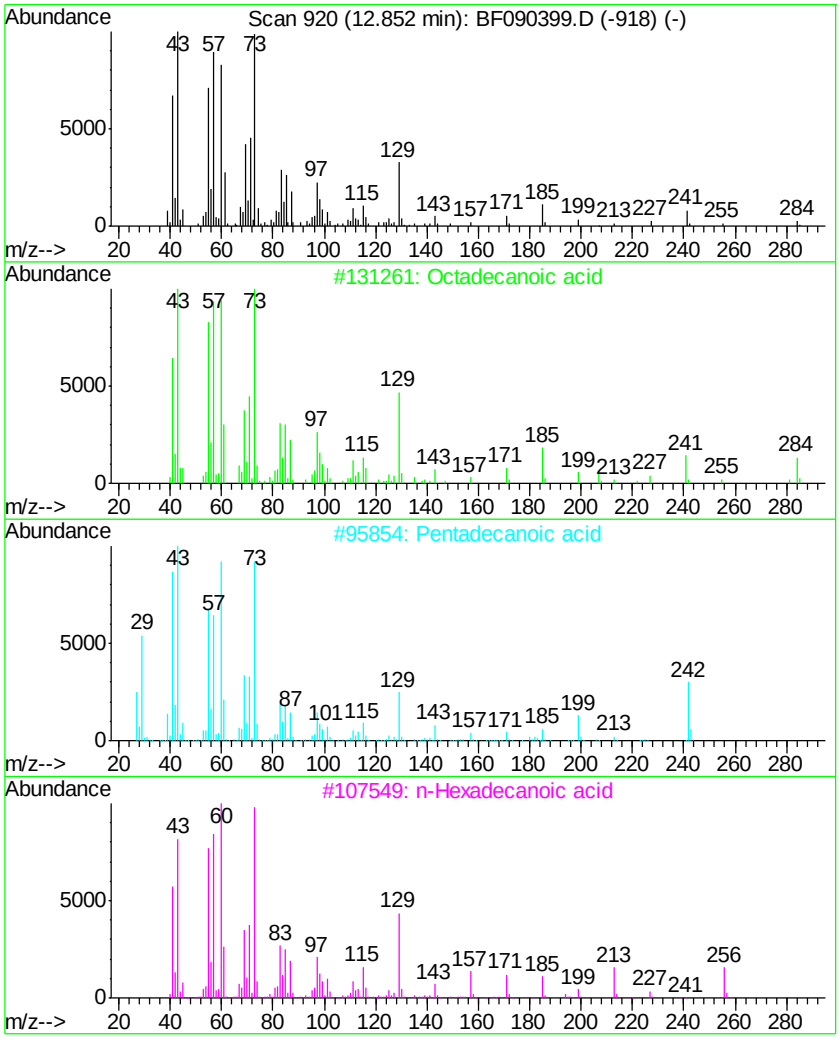
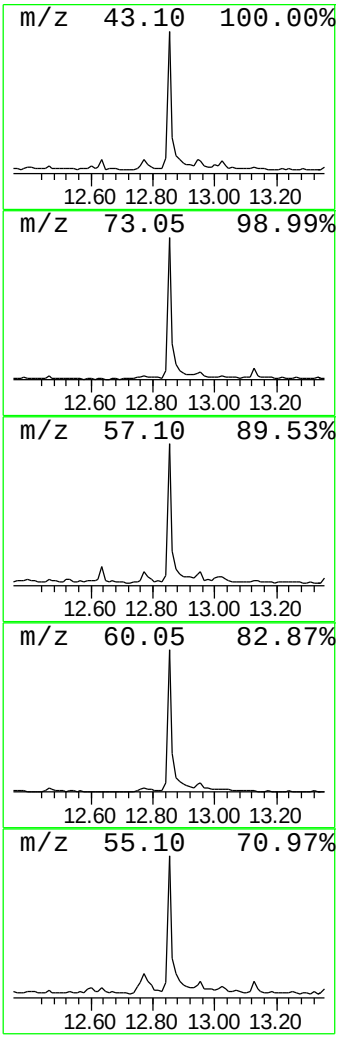
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	4.63 ng	440526	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	38
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	30





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Instrument : BNA_F
ClientSampleId : SUP-B003-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
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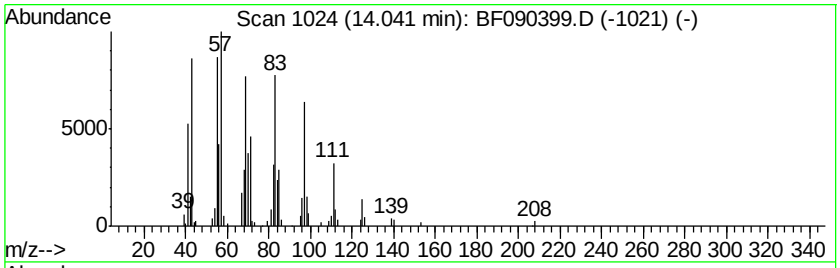
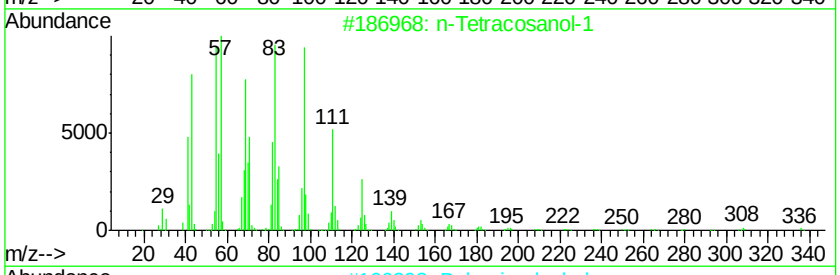
****

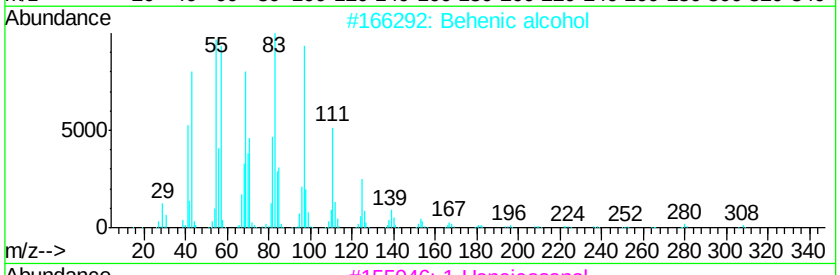
Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

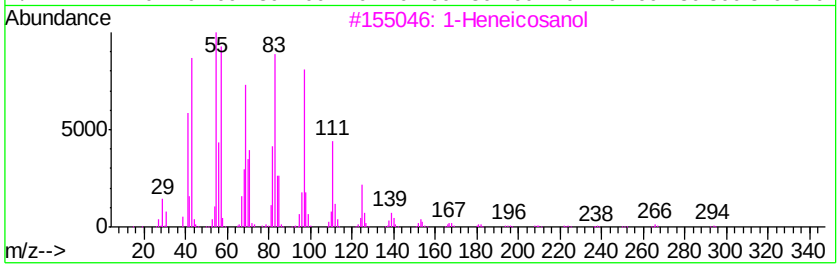
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	5.21 ng	378915	Chrysene-d12	14.19

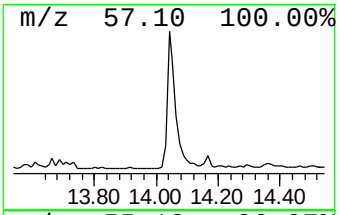
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91

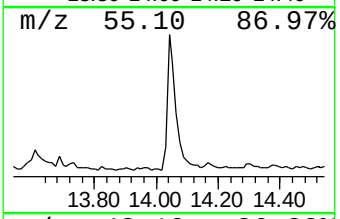


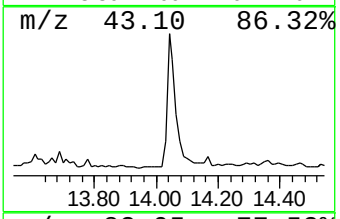


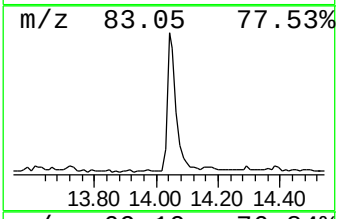


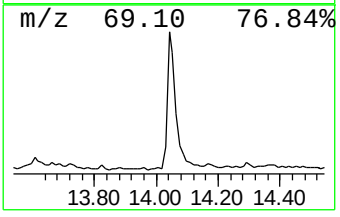












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

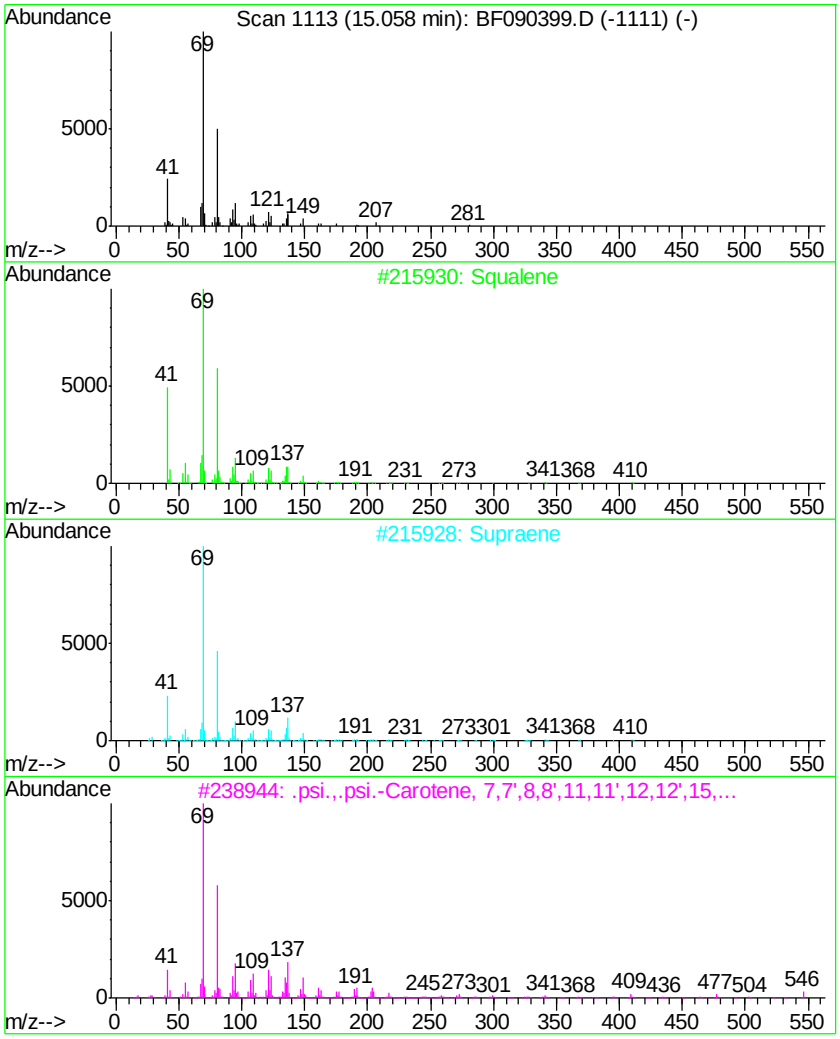
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

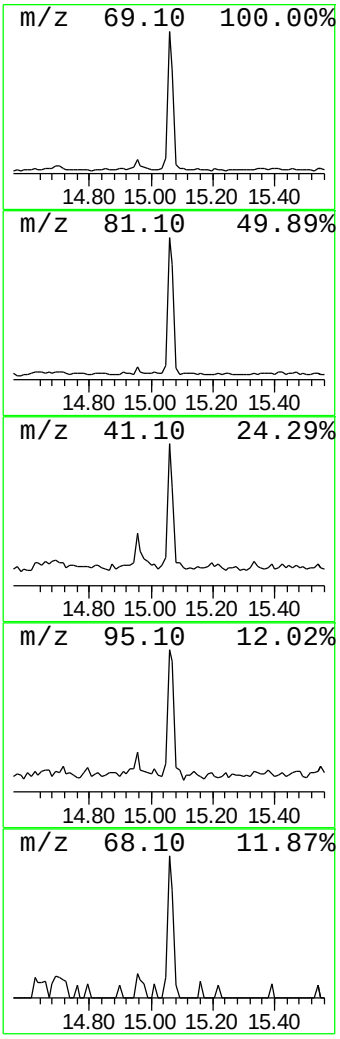
****

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.34 ng	124053	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100516\
Data File : BF090399.D
Acq On : 6 Oct 2016 00:12
Operator : UM/SJ
Sample : H5061-17
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Instrument : BNA_F
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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
unknown3.46	3.46	4.0	ng	286929	1	7.00	1439160	20.0
2-Pentanone, 4-hy...	5.21	19.1	ng	1373130	1	7.00	1439160	20.0
unknown6.77	6.77	86.5	ng	6220800	1	7.00	1439160	20.0
n-Hexadecanoic acid	12.06	7.6	ng	726509	4	11.54	1902900	20.0
Octadecanoic acid	12.85	4.6	ng	440526	4	11.54	1902900	20.0
n-Tetracosanol-1	14.04	5.2	ng	378915	5	14.19	1453520	20.0
Squalene	15.06	2.3	ng	124053	6	15.69	1059500	20.0