LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097048.D
Acq On : 26 Jul 2017 00:07
Operator : SJ/JU
Sample : I4359-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

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-BF072517.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	2.675	131	134	149	rBV	52036	137892	4.18%	0.525%
2	4.651	466	470	482	rVB	223081	379802	11.50%	1.446%
3	5.104	542	547	560	rBV	2973788	3302614	100.00%	12.571%
4	6.169	722	728	741	rBV	2735792	3262547	98.79%	12.419%
5	6.275	741	746	749	rBV	3028644	3015854	91.32%	11.480%
6	6.498	780	784	789	rBV	961562	812931	24.61%	3.094%
7	6.657	806	811	814	rBV	2435712	2268731	68.70%	8.636%
8	6.922	850	856	860	rBV	54201	50129	1.52%	0.191%
9	7.069	876	881	884	rBV	1971810	1994023	60.38%	7.590%
10	7.781	998	1002	1006	rBV	1346925	1090400	33.02%	4.151%
11	8.863	1180	1186	1189	rBV	3132276	2906113	87.99%	11.062%
12	9.257	1249	1253	1258	rBV	353424	266937	8.08%	1.016%
13	9.528	1295	1299	1302	rBV	1064328	948288	28.71%	3.610%
14	9.981	1373	1376	1379	rVB	72722	54251	1.64%	0.207%
15	10.198	1408	1413	1416	rBV	26437	38360	1.16%	0.146%
16	10.310	1428	1432	1436	rBV	1365626	1397868	42.33%	5.321%
17	10.451	1453	1456	1462	rBV	97267	110713	3.35%	0.421%
18	10.898	1523	1532	1534	rBV2	49390	52438	1.59%	0.200%
19	10.998	1545	1549	1553	rBV	925450	739267	22.38%	2.814%
20	11.557	1640	1644	1647	rBV	138013	126504	3.83%	0.482%
21	12.586	1814	1819	1822	rBV	1812257	1783370	54.00%	6.788%
22	13.492	1968	1973	1979	rBV	145325	170197	5.15%	0.648%
23	13.621	1991	1995	2000	rBV	626566	586078	17.75%	2.231%
24	14.121	2078	2080	2086	rBV	40040	50410	1.53%	0.192%
25	14.704	2176	2179	2185	rBV2	30949	50166	1.52%	0.191%
26	14.968	2220	2224	2230	rBV	472308	532429	16.12%	2.027%
27	15.380	2290	2294	2298	rBV	40472	65539	1.98%	0.249%
28	16.662	2506	2512	2518	rBV10	32514	77501	2.35%	0.295%

Sum of corrected areas: 26271352

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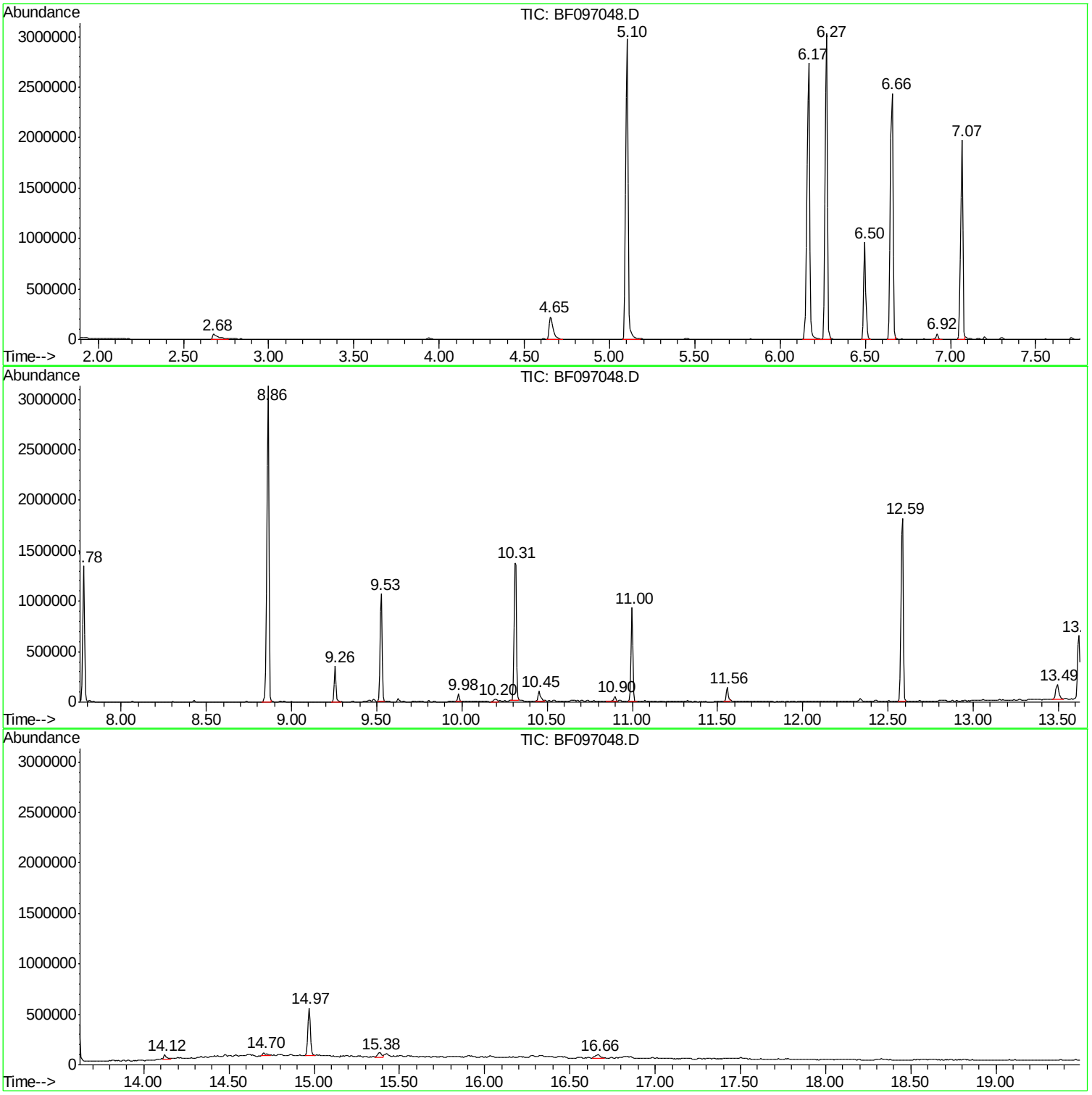
Instrument :
BNA_F
ClientSampleId :
CEMETERY-7-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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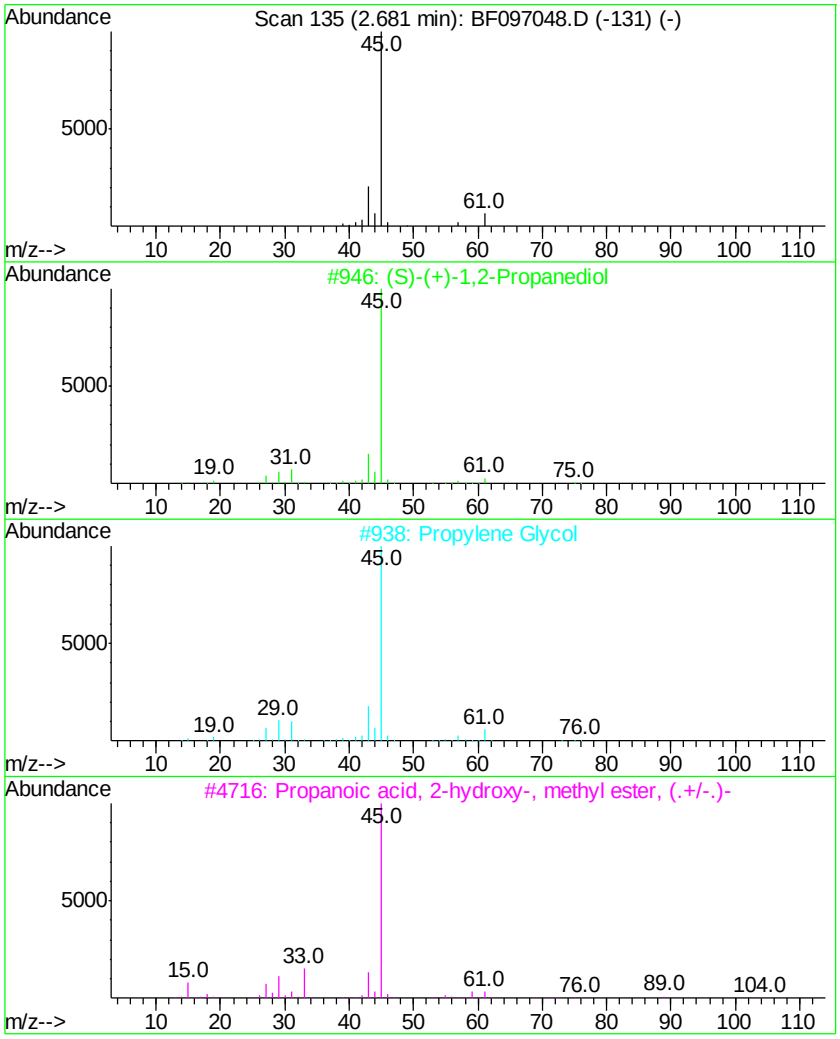
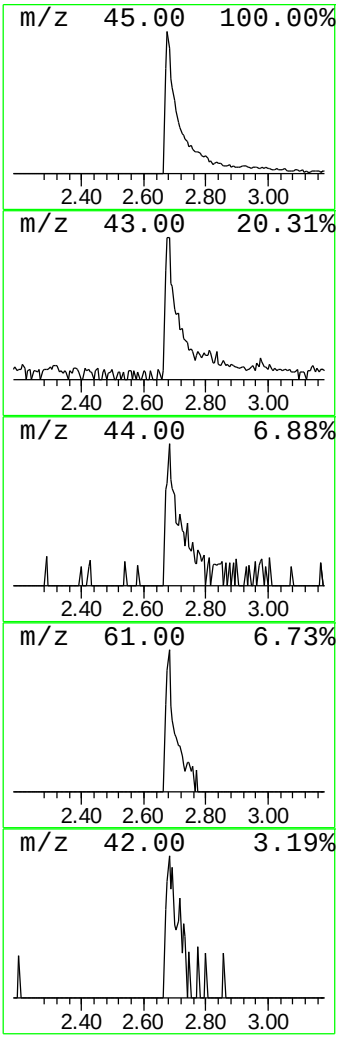
Peak Number 1 unknown2.68 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.68	3.39 ng	137892	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	7





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Misc :
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Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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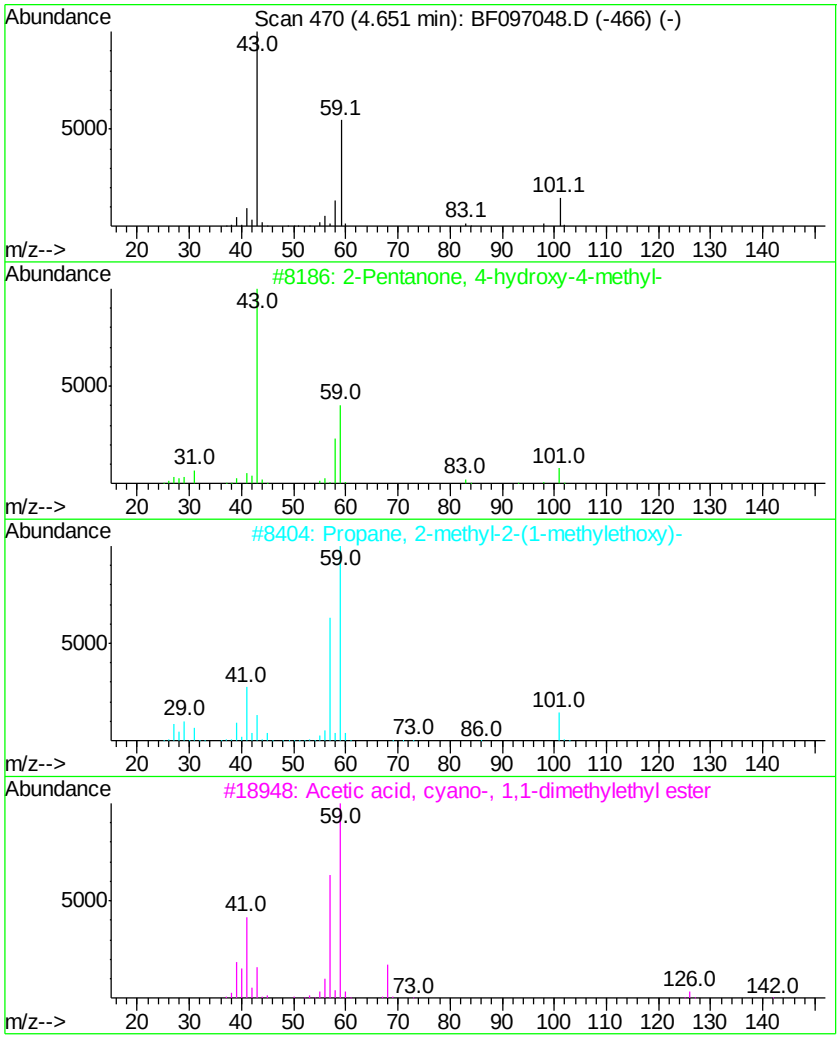
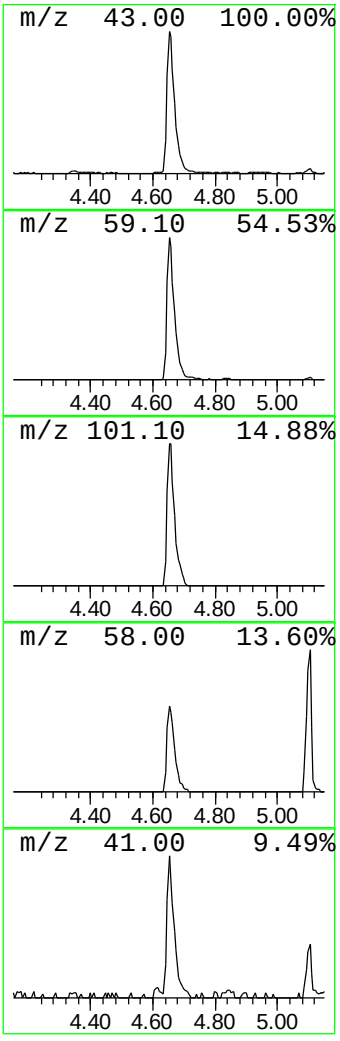
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	9.34 ng	379802	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Integration Parameters: LSCINT.P

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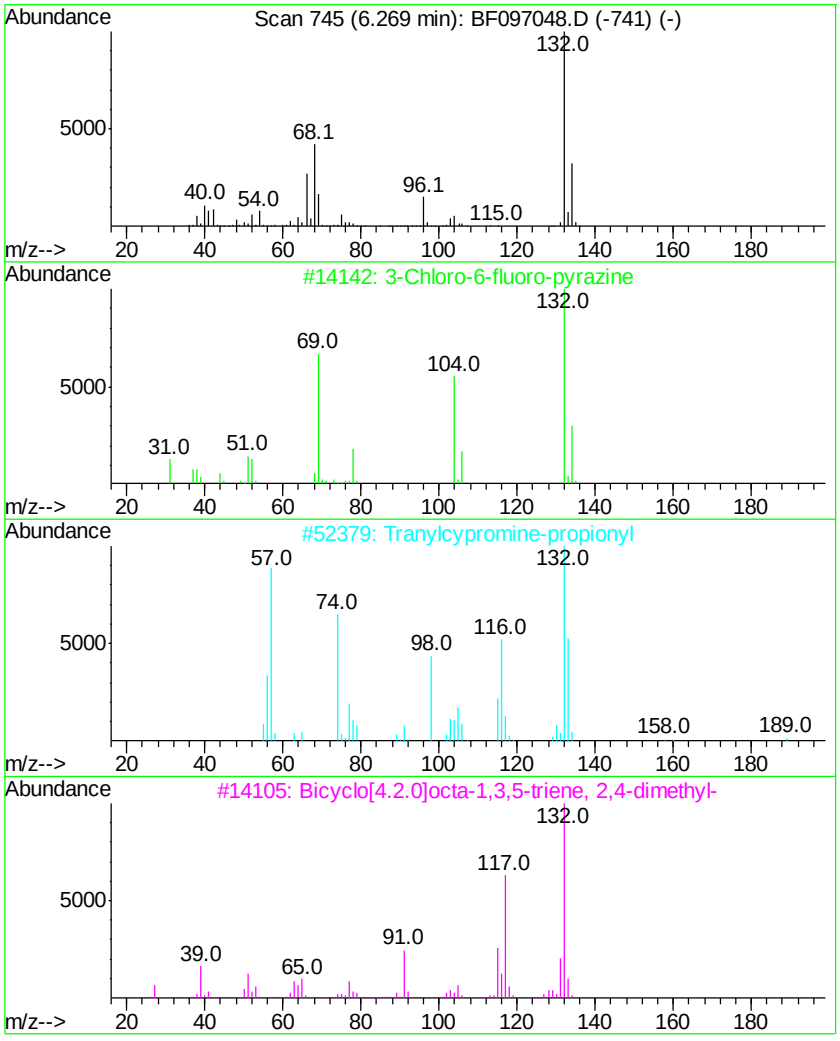
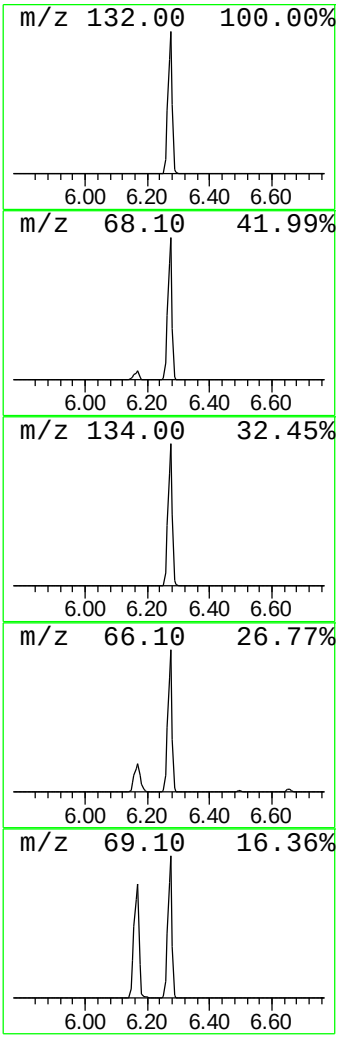
Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	74.20 ng	3015850	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

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TIC Library : C:\DATABASE\NIST11.L
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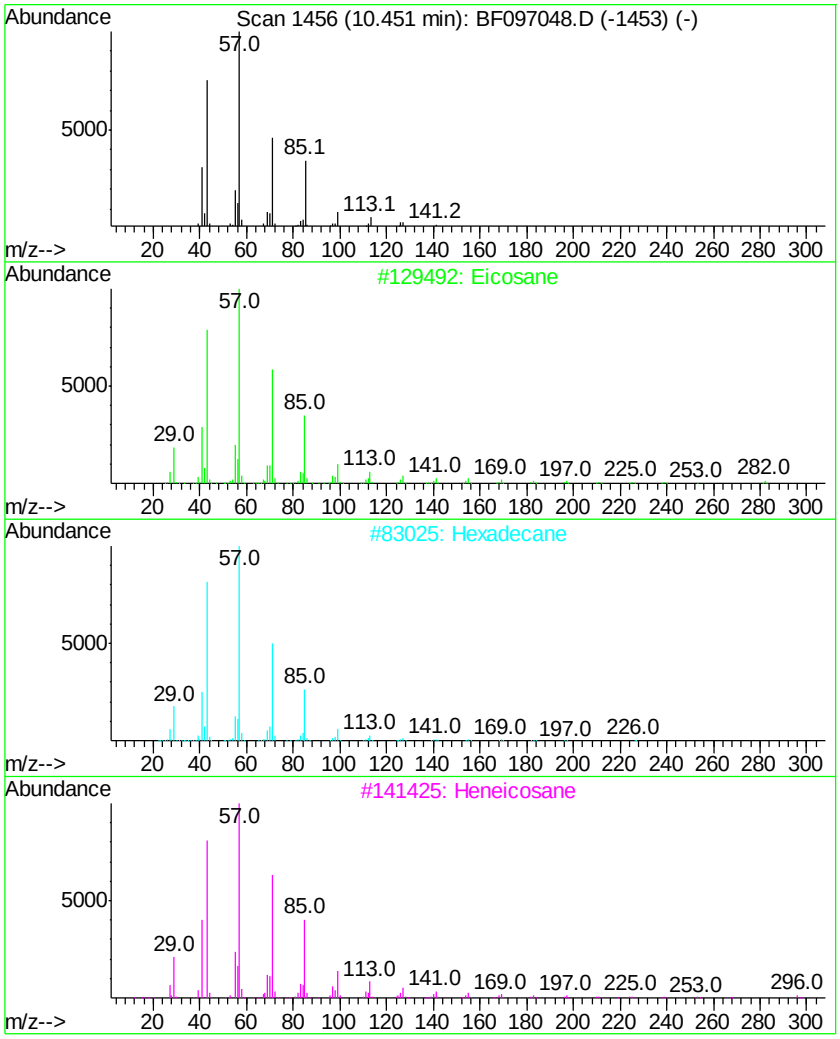
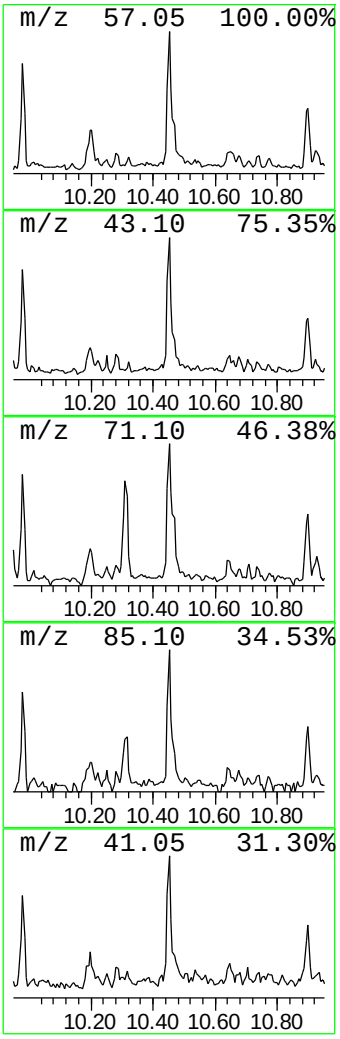
****

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	3.00 ng	110713	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	80
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
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Acq On : 26 Jul 2017 00:07
Operator : SJ/JU
Sample : I4359-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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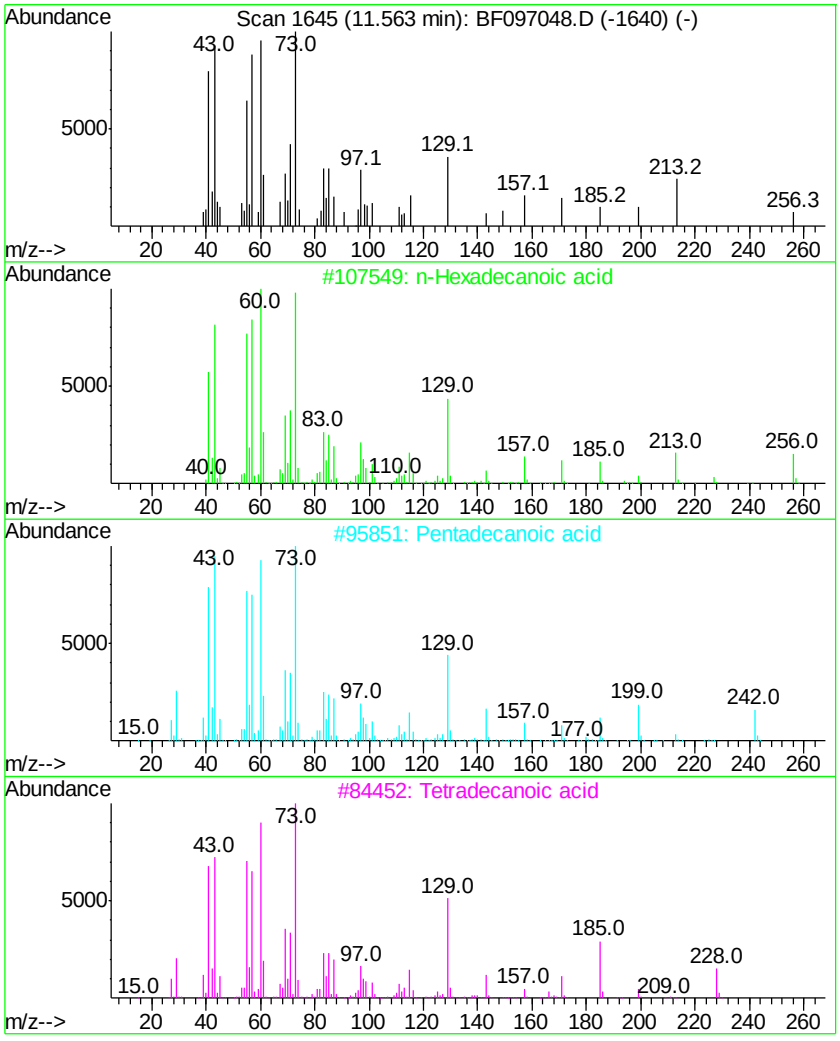
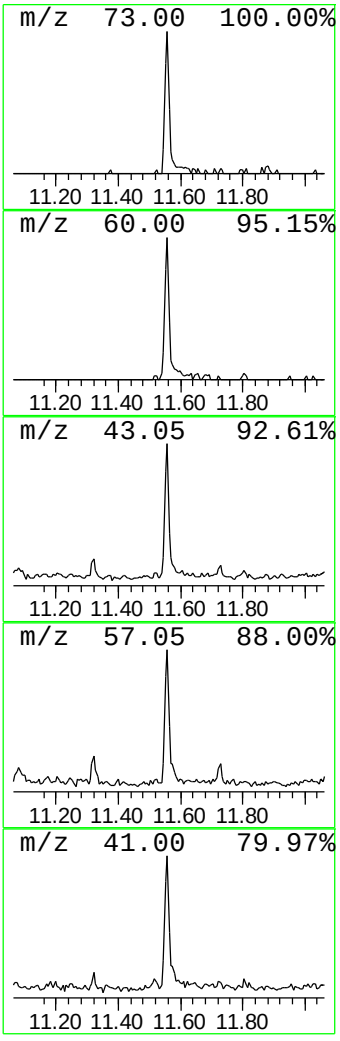
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	3.42 ng	126504	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Trehalose	342	C12H22O11	000099-20-7	47





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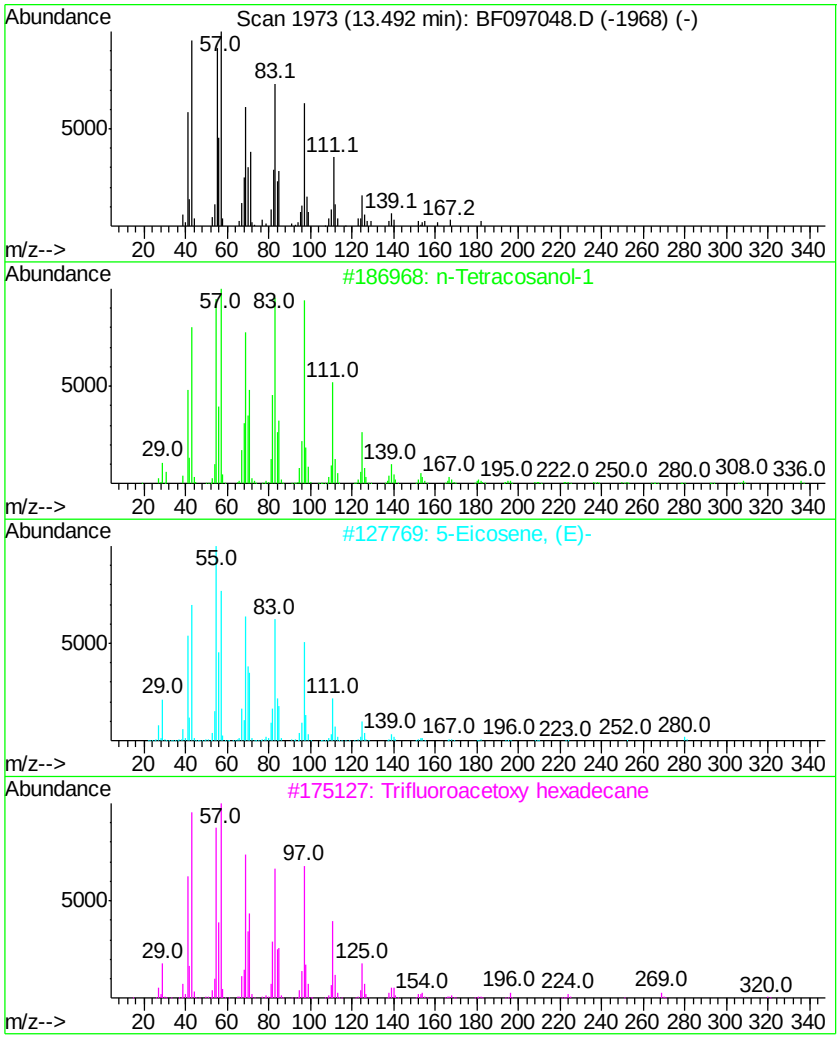
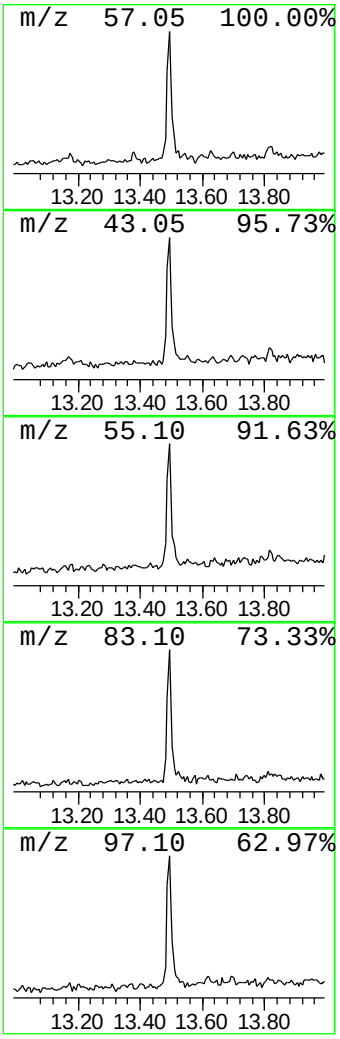
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	5.81 ng	170197	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Docosene	308	C22H44	001599-67-3	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

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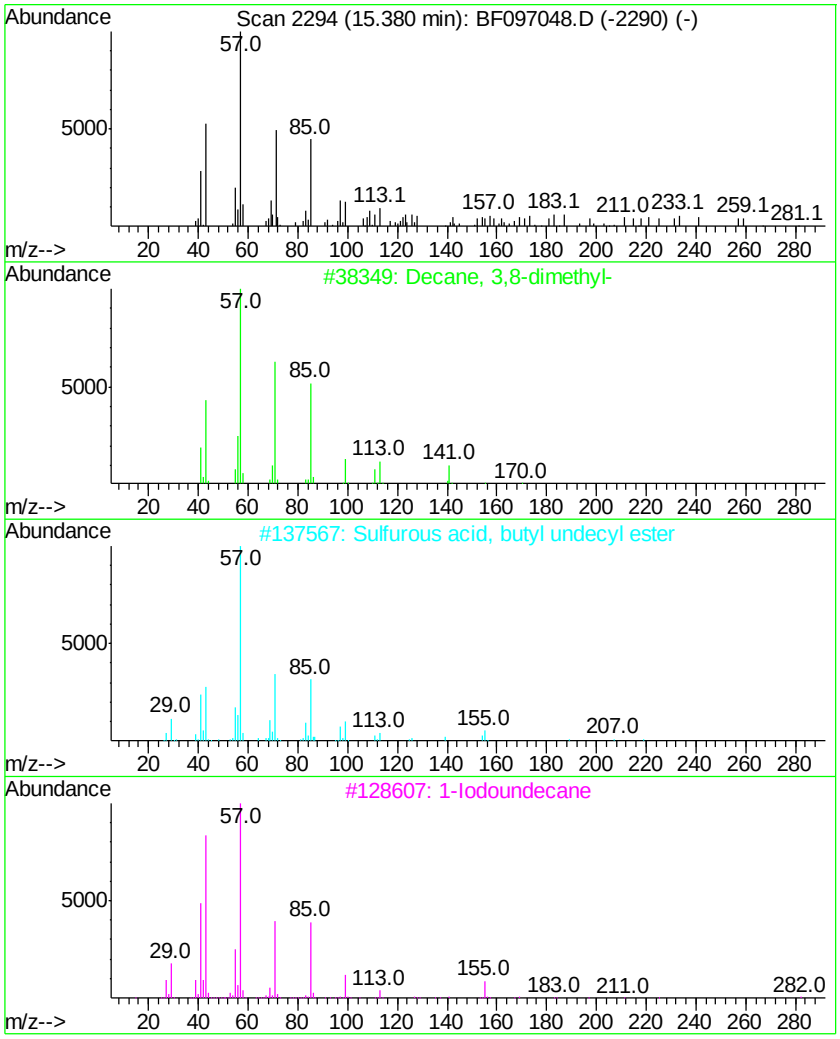
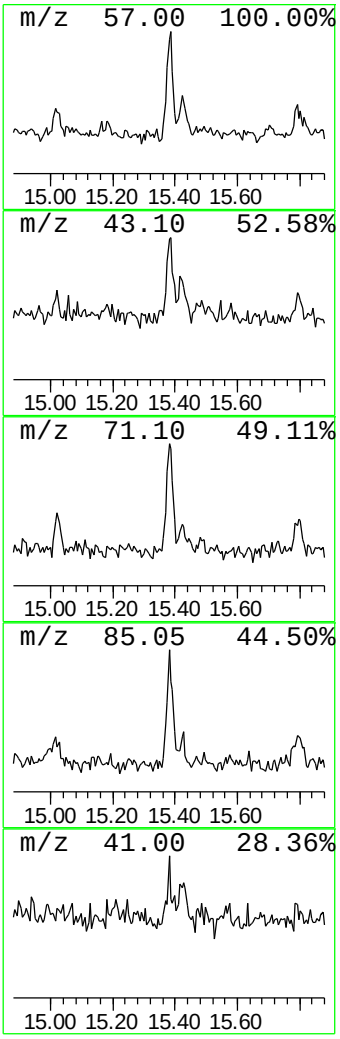
Peak Number 8 Decane, 3,8-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	2.46 ng	65539	Perylene-d12	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
2	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
3	1-Iodoundecane	282	C11H23I	004282-44-4	59
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59





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TIC Library : C:\DATABASE\NIST11.L
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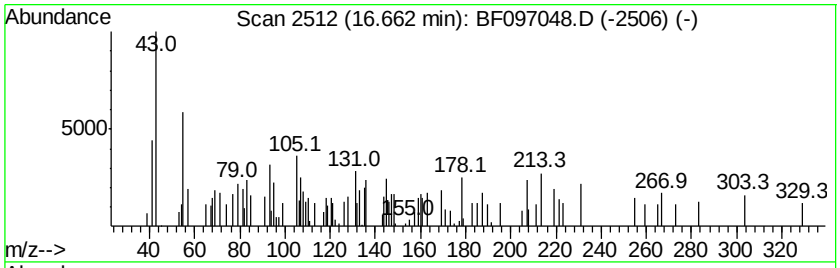
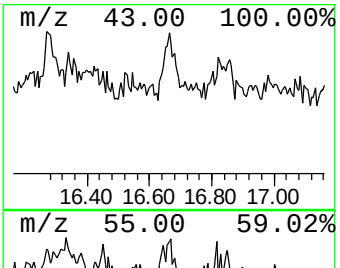
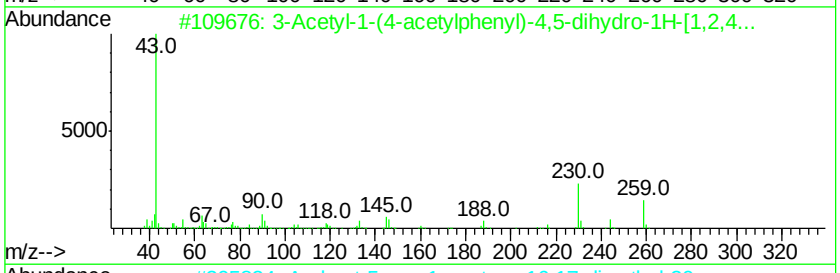
Peak Number 9 unknown16.66 Concentration Rank 8

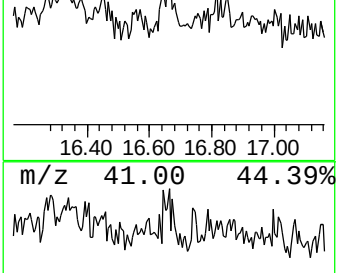
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.91 ng	77501	Perylene-d12	14.97

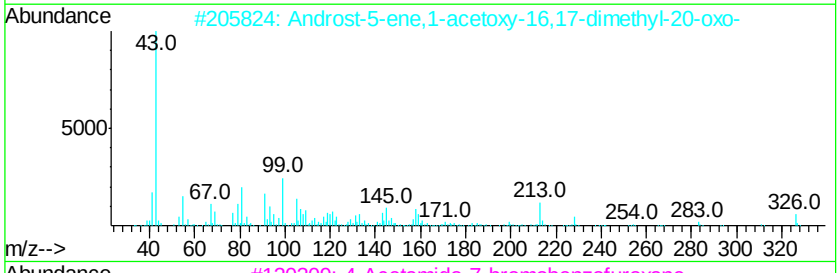
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Acetyl-1-(4-acetylphenyl)-4,5-...	259	C13H13N3O3	139455-69-9	9
2	Androst-5-ene,1-acetoxy-16,17-di...	386	C25H38O3	294866-91-4	9
3	4-Acetamido-7-bromobenzofuroxane	271	C8H6BrN3O3	1000140-65-2	4
4	Ethyl 3-bromo-4,6-dimethyl-2H-py...	274	C10H11BrO4	018152-79-9	1
5	1-Methoxy-3,4-dimethyl-1-phenyl-...	264	C13H18GeO	026311-84-2	1

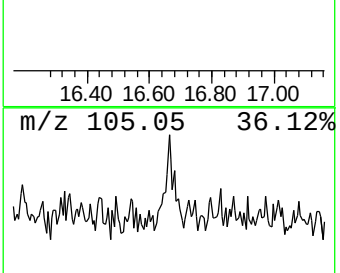


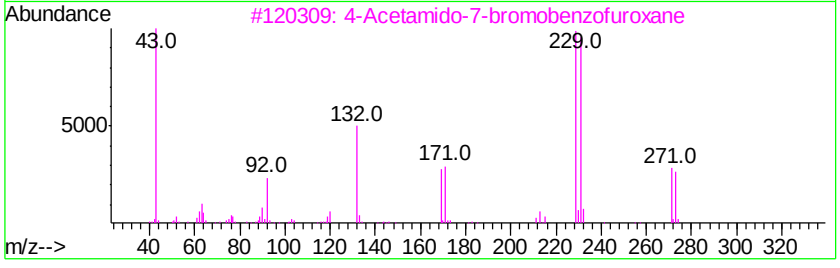


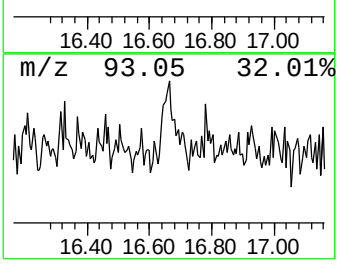












Tentatively Identified Compound (LSC) summary

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Data File : BF097048.D
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-7-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
unknown2.68	2.68	3.4	ng	137892	1	6.50	812931	20.0
2-Pentanone, 4-hy...	4.65	9.3	ng	379802	1	6.50	812931	20.0
unknown6.27	6.27	74.2	ng	3015850	1	6.50	812931	20.0
Eicosane	10.45	3.0	ng	110713	4	11.00	739267	20.0
n-Hexadecanoic acid	11.56	3.4	ng	126504	4	11.00	739267	20.0
n-Tetracosanol-1	13.49	5.8	ng	170197	5	13.62	586078	20.0
Decane, 3,8-dimet...	15.38	2.5	ng	65539	6	14.97	532429	20.0
unknown16.66	16.66	2.9	ng	77501	6	14.97	532429	20.0