LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096847.D
Acq On : 18 Jul 2017 14:53
Operator : SJ/JU
Sample : I4223-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC071417-1N

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-BF071317.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	2.887	151	153	164	rBV	44396	88982	2.36%	0.295%
2	4.787	472	476	491	rVB	238169	396265	10.50%	1.312%
3	5.216	543	549	552	rBV	3092145	3426936	90.83%	11.348%
4	6.257	719	726	729	rBV	2753697	3377335	89.52%	11.184%
5	6.375	740	746	749	rBV	2947655	3210619	85.10%	10.632%
6	6.598	780	784	787	rBV	702161	615374	16.31%	2.038%
7	6.757	806	811	814	rBV	2410762	2442376	64.73%	8.088%
8	7.163	874	880	883	rBV	1936821	2181795	57.83%	7.225%
9	7.287	892	901	905	rBV	69322	98815	2.62%	0.327%
10	7.798	985	988	993	rBV	40334	37947	1.01%	0.126%
11	7.881	997	1002	1005	rBV	978328	951262	25.21%	3.150%
12	8.957	1179	1185	1189	rBV	3240564	3772906	100.00%	12.494%
13	9.351	1247	1252	1255	rBV	756721	612025	16.22%	2.027%
14	9.628	1293	1299	1302	rBV	1011382	933948	24.75%	3.093%
15	10.416	1427	1433	1436	rBV	2038880	2171531	57.56%	7.191%
16	10.545	1452	1455	1465	rVB	75653	81076	2.15%	0.268%
17	10.992	1527	1531	1534	rBV	59914	50550	1.34%	0.167%
18	11.098	1540	1549	1553	rBV	1050621	980352	25.98%	3.246%
19	12.692	1814	1820	1823	rBV	2938351	3341392	88.56%	11.065%
20	13.592	1969	1973	1979	rBV	132078	151909	4.03%	0.503%
21	13.721	1991	1995	1999	rBV	744413	748756	19.85%	2.479%
22	15.092	2223	2228	2233	rBV	422501	475524	12.60%	1.575%
23	15.527	2297	2302	2306	rBV2	35515	51064	1.35%	0.169%

Sum of corrected areas: 30198739

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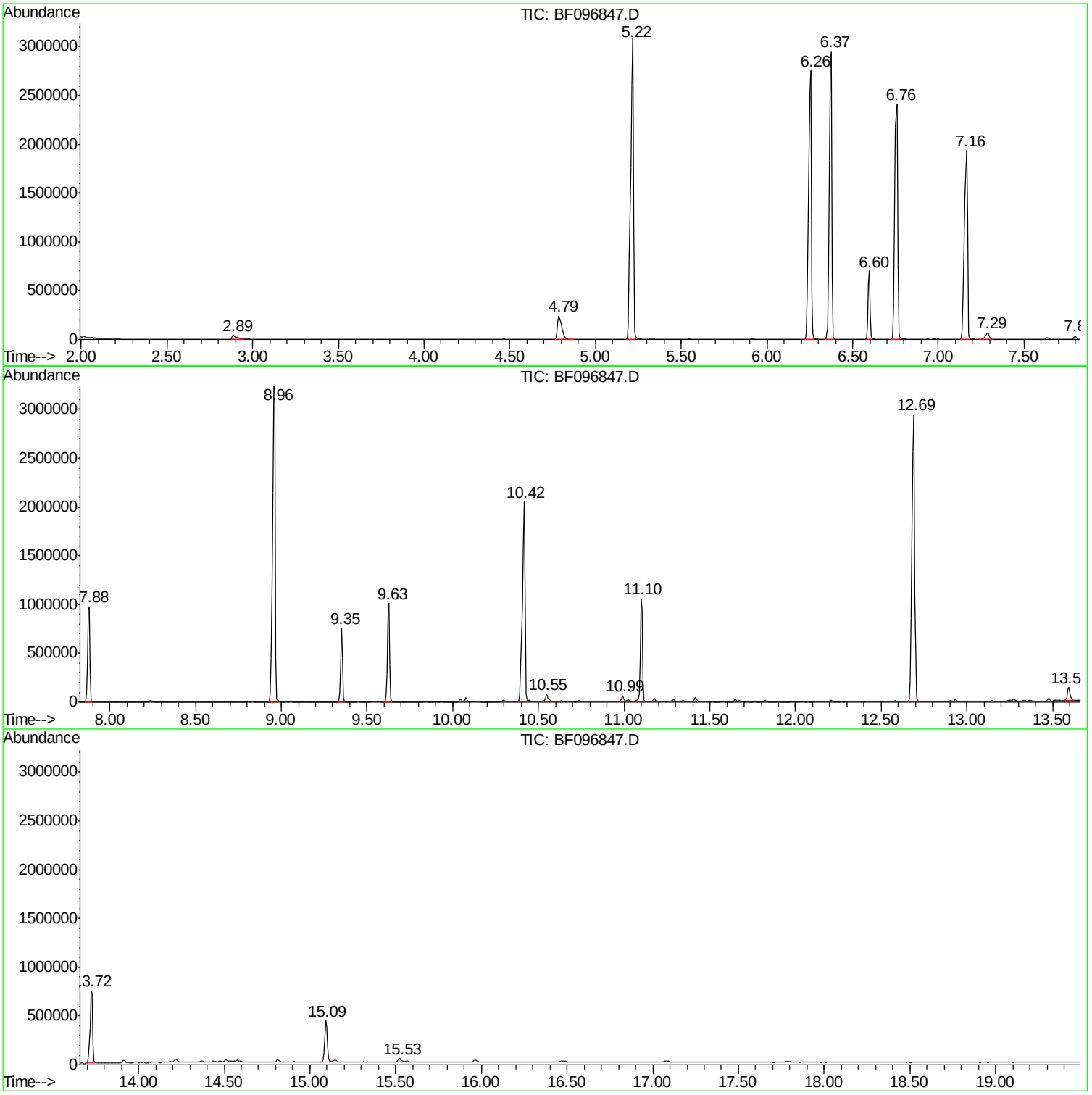
ClientSampleId :
WC071417-1N

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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

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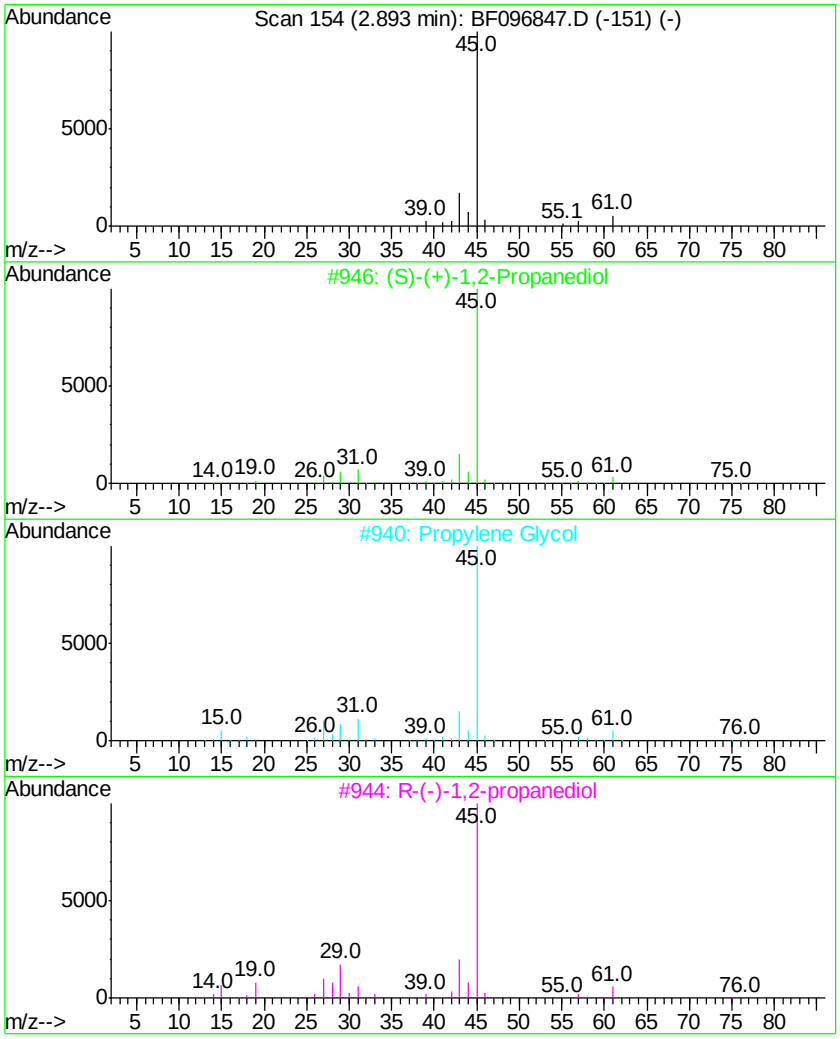
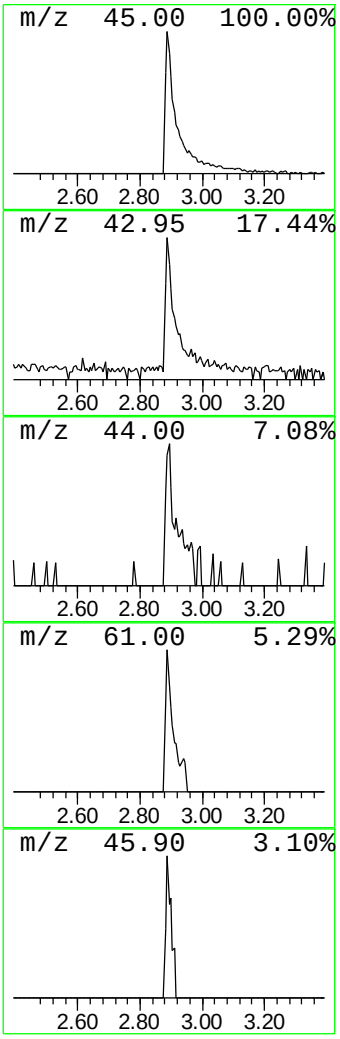
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	2.89 ng	88982	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Formamide	45	CH3NO	000075-12-7	7





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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC071417-1N

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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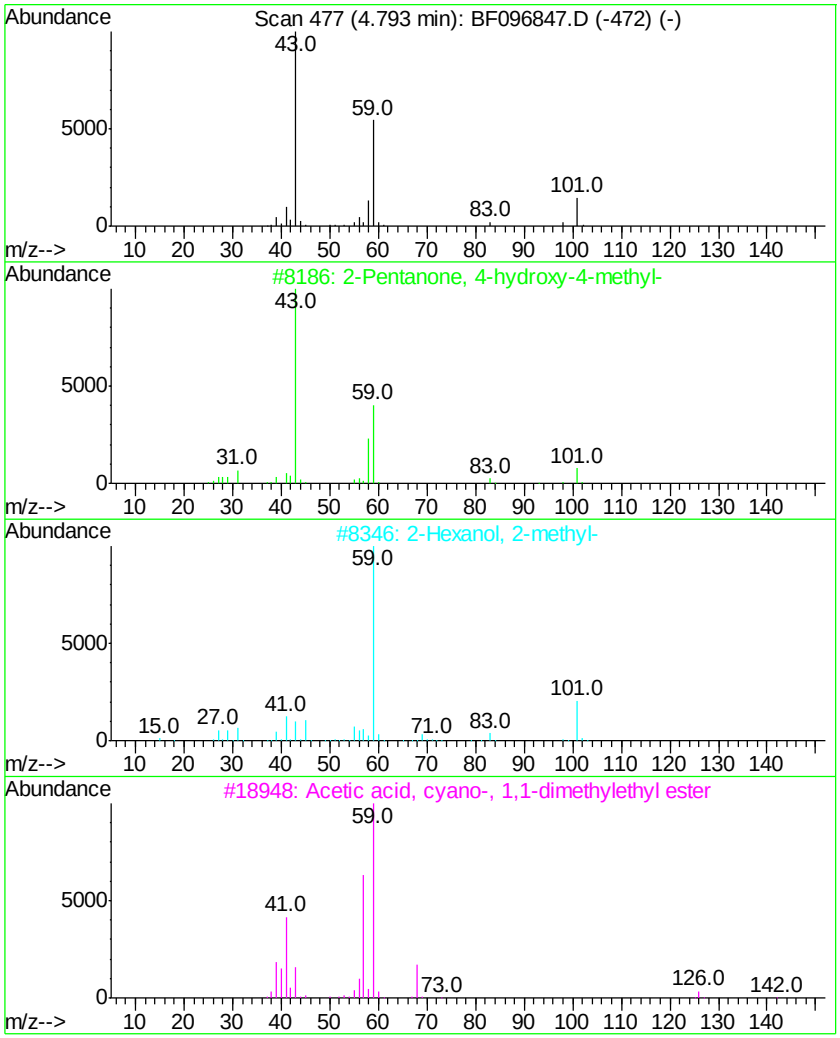
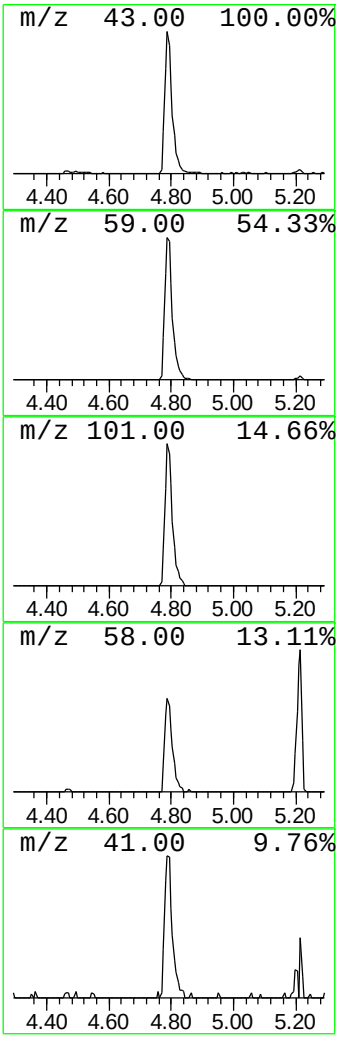
Peak Number 2 unknown4.79 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	12.88 ng	396265	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





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Data File : BF096847.D
Acq On : 18 Jul 2017 14:53
Operator : SJ/JU
Sample : I4223-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC071417-1N

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
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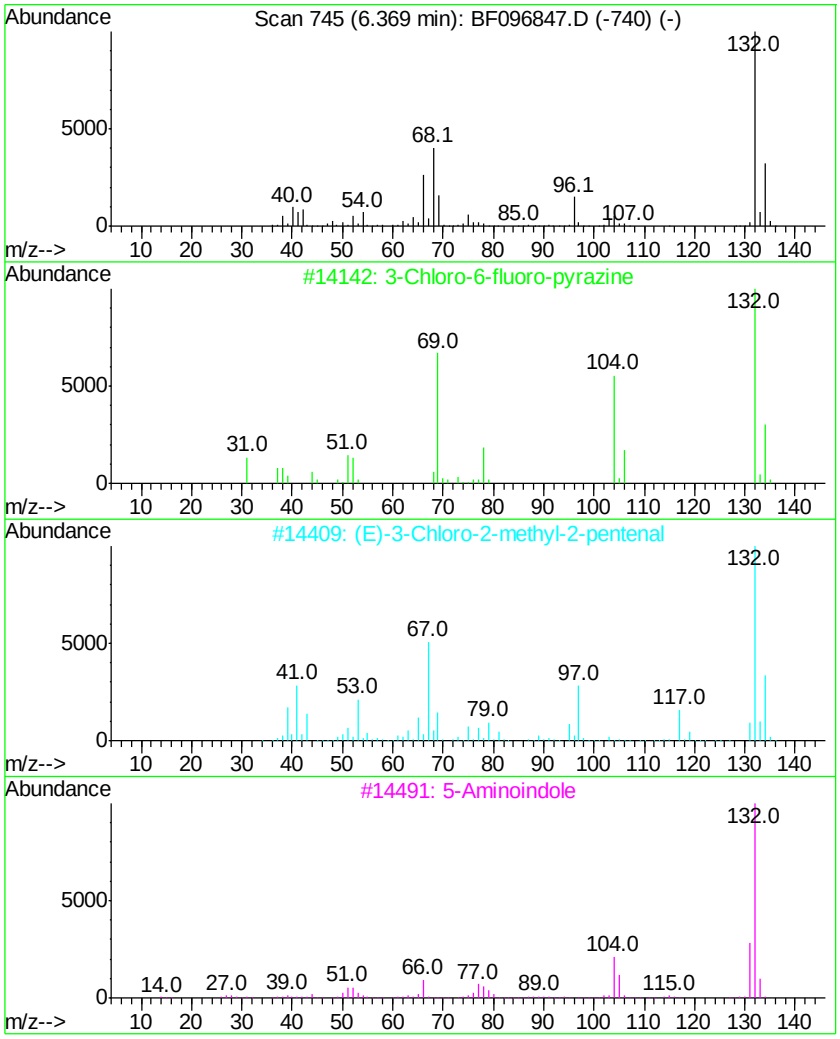
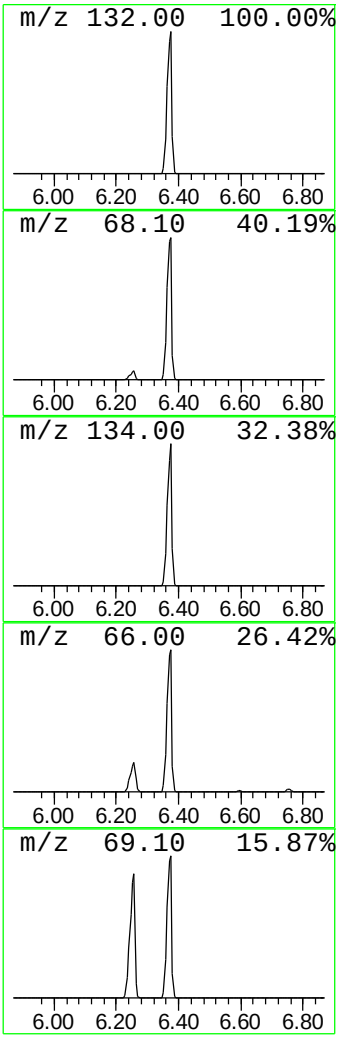
Peak Number 3 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	104.35 ng	3210620	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
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Sample : I4223-01
Misc :
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Instrument : BNA_F
ClientSampleId : WC071417-1N

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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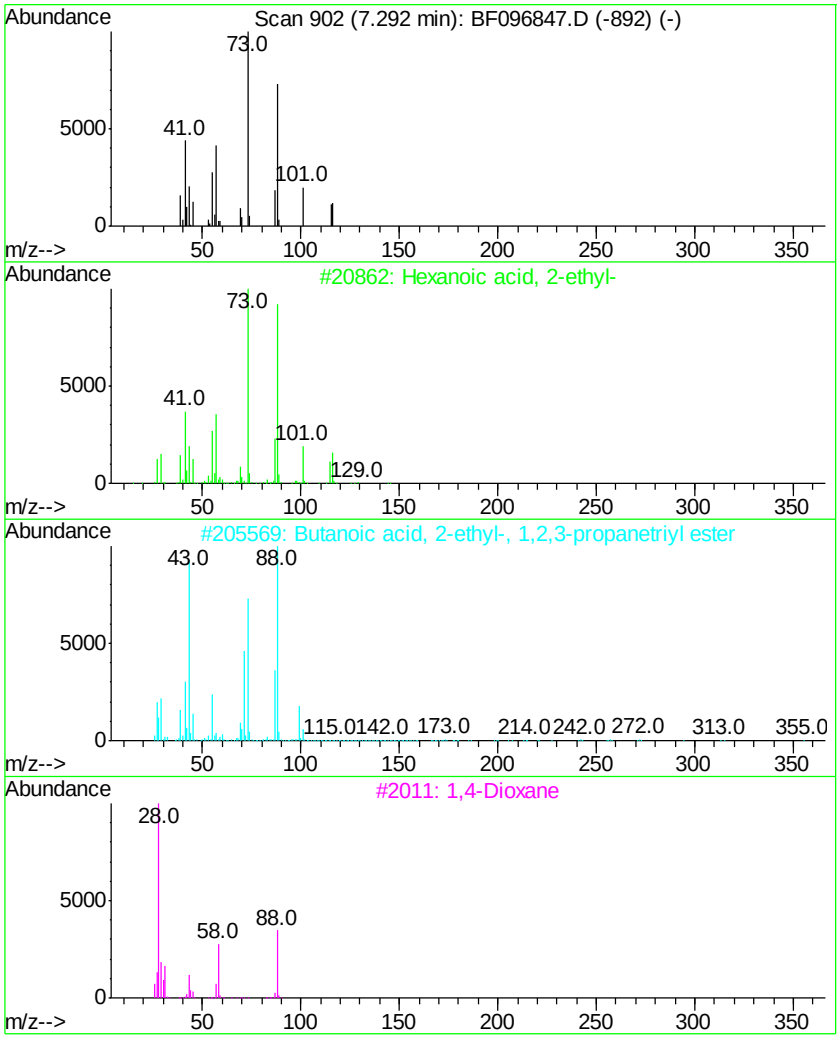
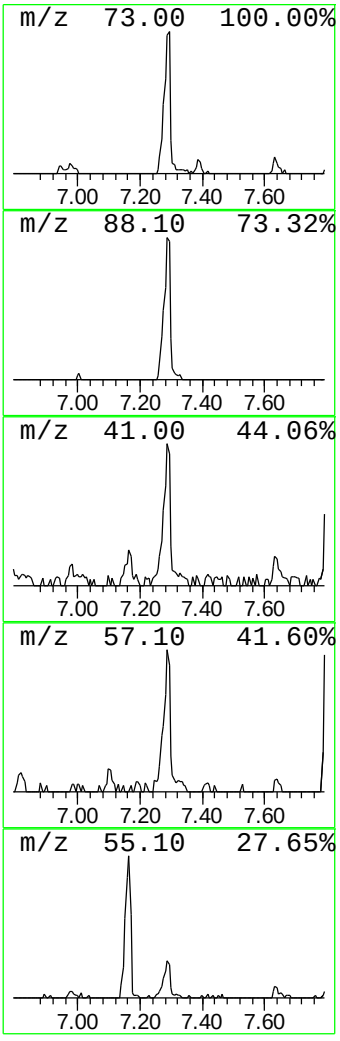
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	2.08 ng	98815	Naphthalene-d8	7.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	1,4-Dioxane	88	C4H8O2	000123-91-1	47
4	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	33
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	035939-74-3	33





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Sample : I4223-01
Misc :
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Instrument : BNA_F
ClientSampleId : WC071417-1N

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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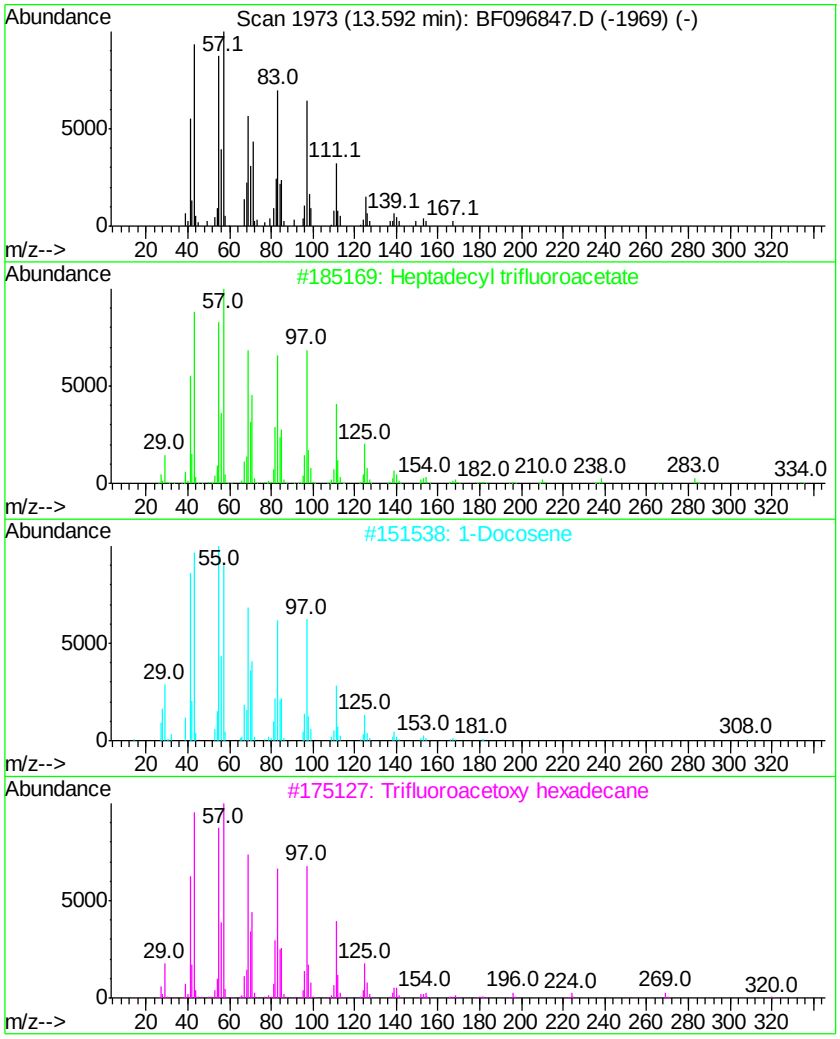
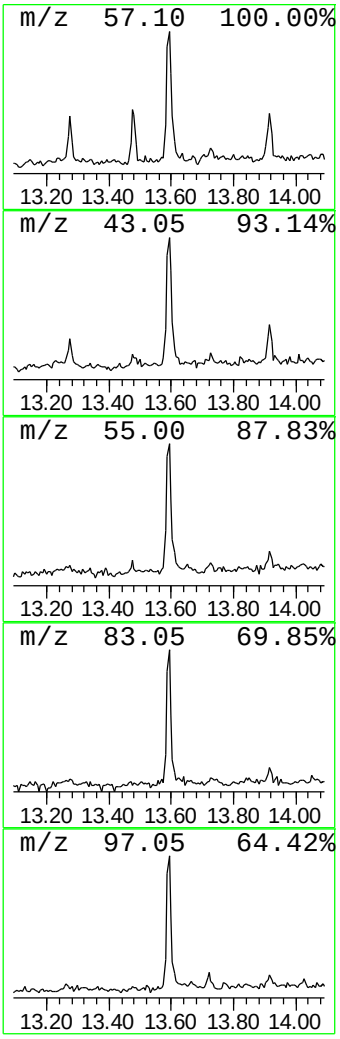
Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.06 ng	151909	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	1-Docosene	308	C22H44	001599-67-3	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Octacosanol	410	C28H58O	000557-61-9	91





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

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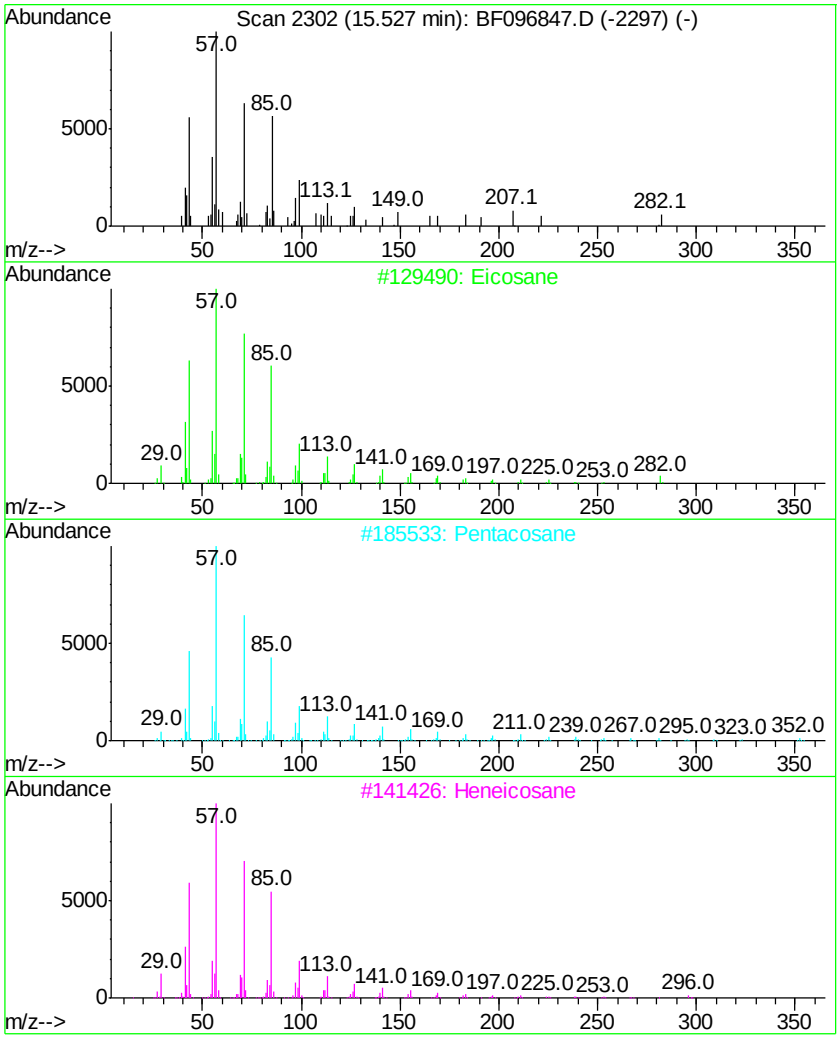
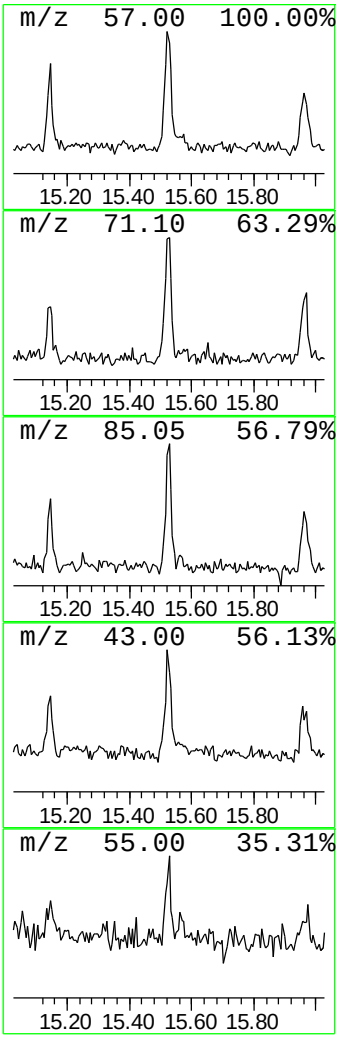
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	2.15 ng	51064	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentacosane	352	C25H52	000629-99-2	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetracontane	563	C40H82	004181-95-7	78
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	2.89	2.9	ng	88982	1	6.60	615374	20.0
unknown4.79	4.79	12.9	ng	396265	1	6.60	615374	20.0
unknown6.37	6.37	104.3	ng	3210620	1	6.60	615374	20.0
Hexanoic acid, 2-...	7.29	2.1	ng	98815	2	7.88	951262	20.0
Heptadecyl triflu...	13.59	4.1	ng	151909	5	13.73	748756	20.0
Eicosane	15.53	2.1	ng	51064	6	15.09	475524	20.0