LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-11B

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-BF122116.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	4.910	245	247	256	rVB	1013498	1190807	12.99%	1.946%
2	5.356	283	286	288	rBV	2886414	3716234	40.55%	6.074%
3	6.396	374	377	379	rBV	2224858	2467307	26.92%	4.033%
4	6.522	385	388	390	rBV	5451371	6646625	72.53%	10.863%
5	6.739	405	407	410	rBV	1277842	1647582	17.98%	2.693%
6	6.899	418	421	424	rVB	4891702	5802754	63.32%	9.484%
7	7.310	454	457	460	rBV	3487000	5268452	57.49%	8.611%
8	8.030	517	520	523	rBV	2409129	2301178	25.11%	3.761%
9	9.116	611	615	617	rBV	7012882	9164423	100.00%	14.978%
10	9.505	647	649	654	rVB	165888	154465	1.69%	0.252%
11	9.779	670	673	676	rBV	2510112	2673509	29.17%	4.370%
12	10.568	739	742	745	rBV2	3467492	5222772	56.99%	8.536%
13	10.693	751	753	760	rVB	102118	129117	1.41%	0.211%
14	11.265	800	803	805	rBV	2752331	2659139	29.02%	4.346%
15	11.802	848	850	854	rBV2	135252	193956	2.12%	0.317%
16	12.591	917	919	924	rBV	188621	278046	3.03%	0.454%
17	12.682	924	927	929	rVV	205391	206226	2.25%	0.337%
18	12.854	939	942	944	rBV	6607970	7111131	77.59%	11.622%
19	13.379	986	988	990	rBV	101050	108159	1.18%	0.177%
20	13.757	1018	1021	1027	rVB	114248	163903	1.79%	0.268%
21	13.894	1030	1033	1036	rBV	2247139	2137948	23.33%	3.494%
22	15.288	1152	1155	1158	rBV	1213638	1666391	18.18%	2.724%
23	15.334	1158	1159	1166	rVB2	91346	119331	1.30%	0.195%
24	16.180	1230	1233	1241	rVB2	74373	155897	1.70%	0.255%

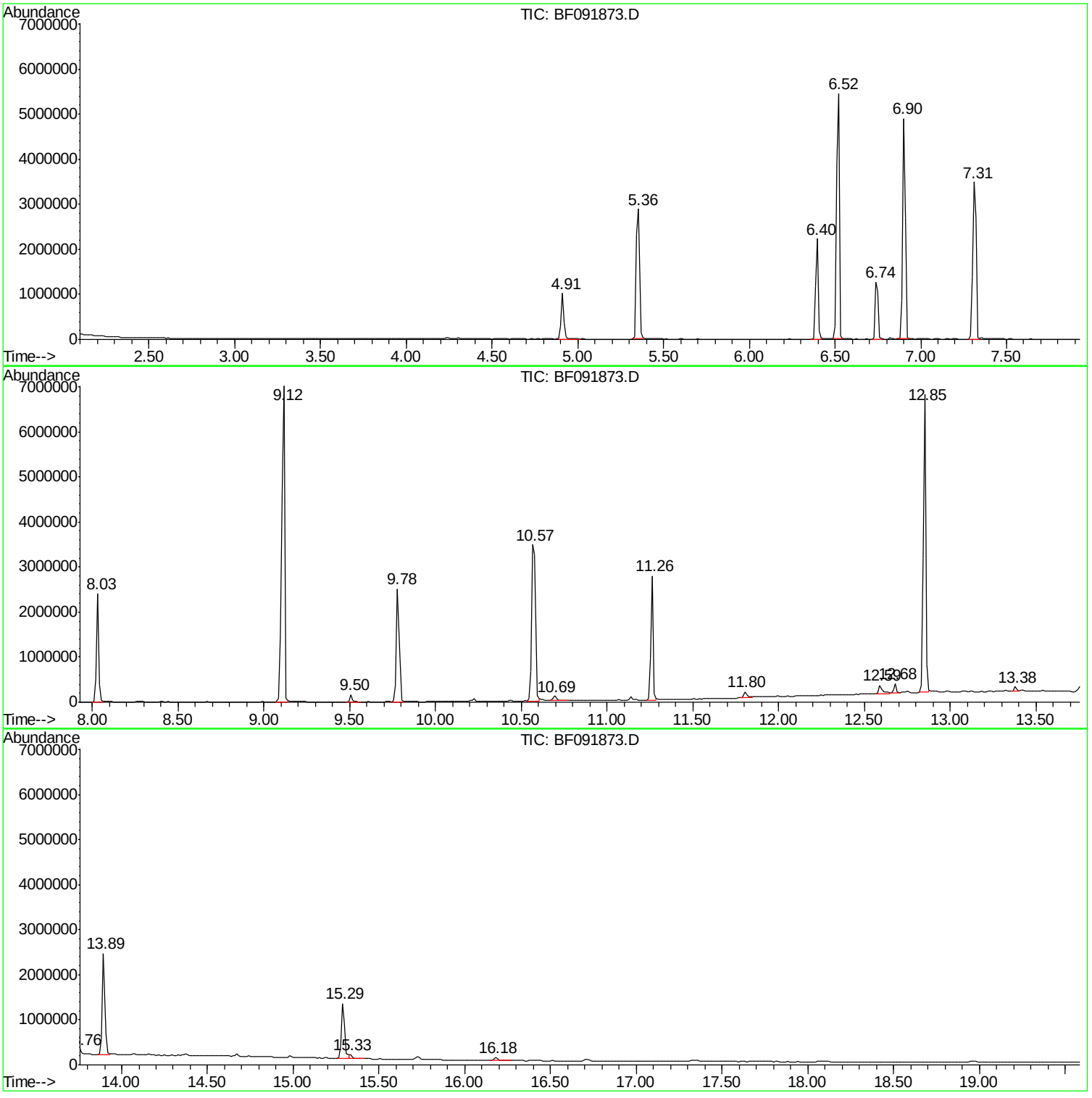
Sum of corrected areas: 61185352

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

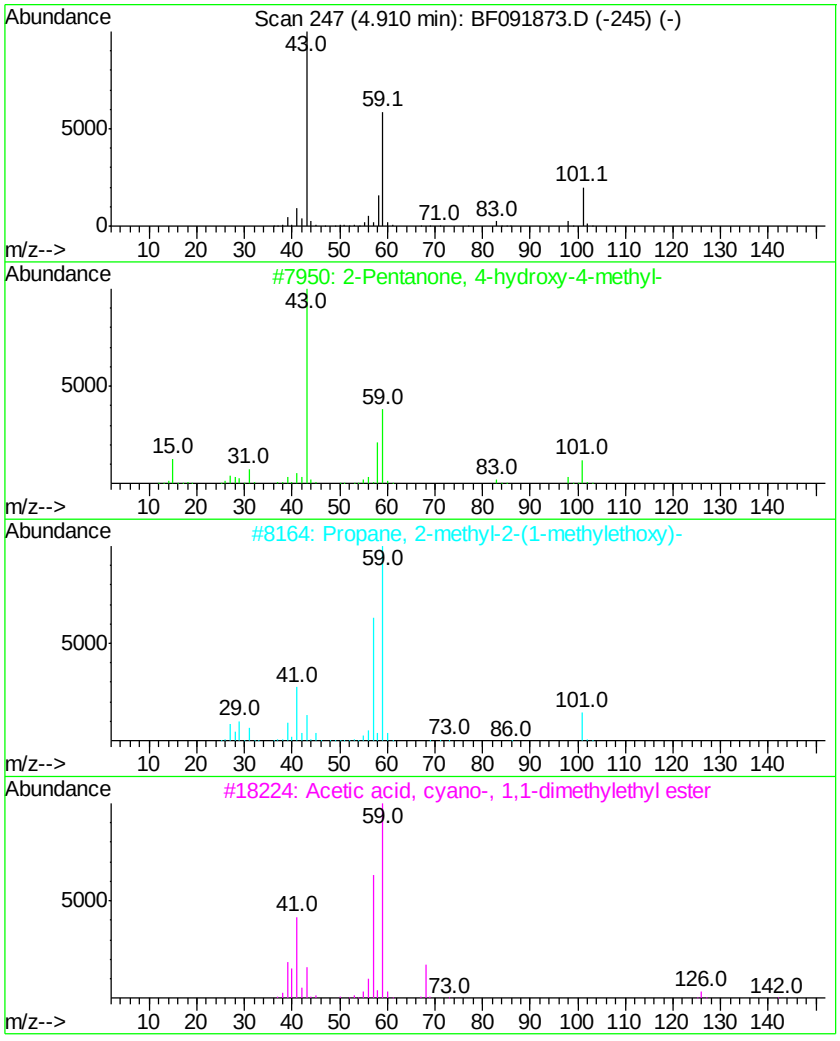
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

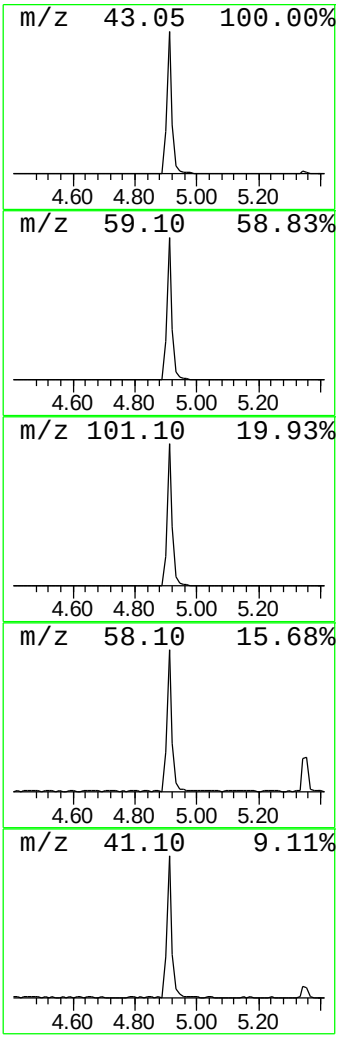
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	14.46 ng	1190810	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

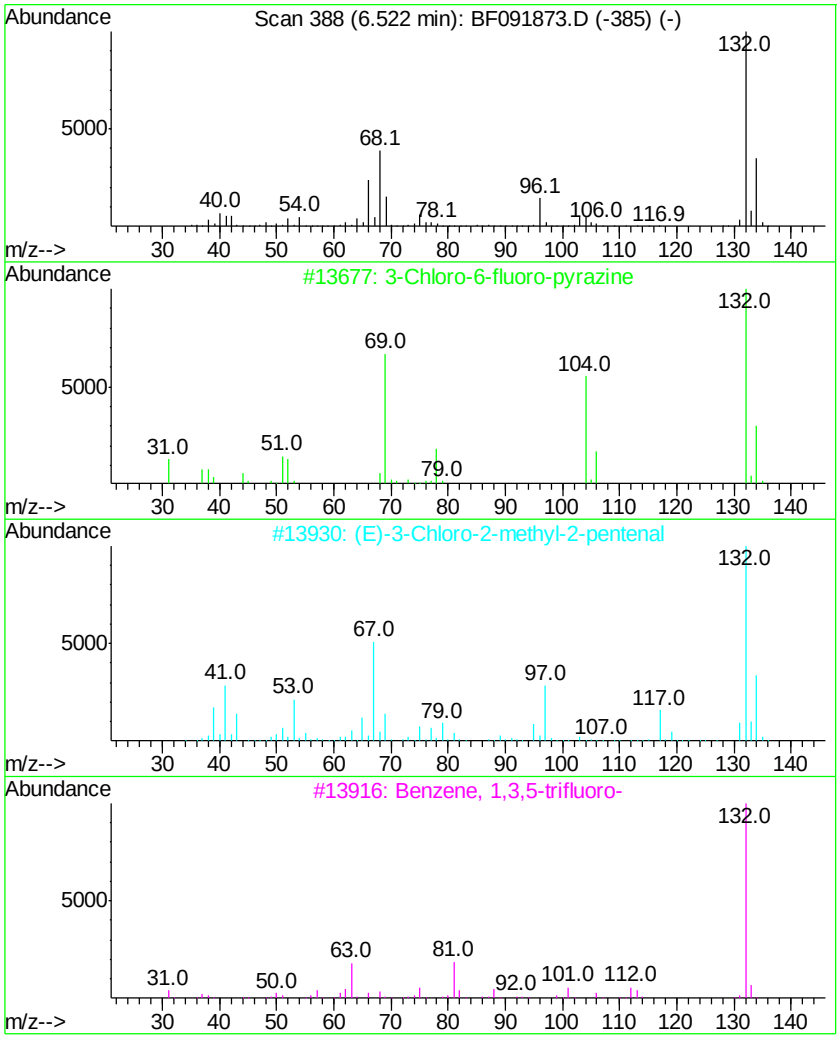
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

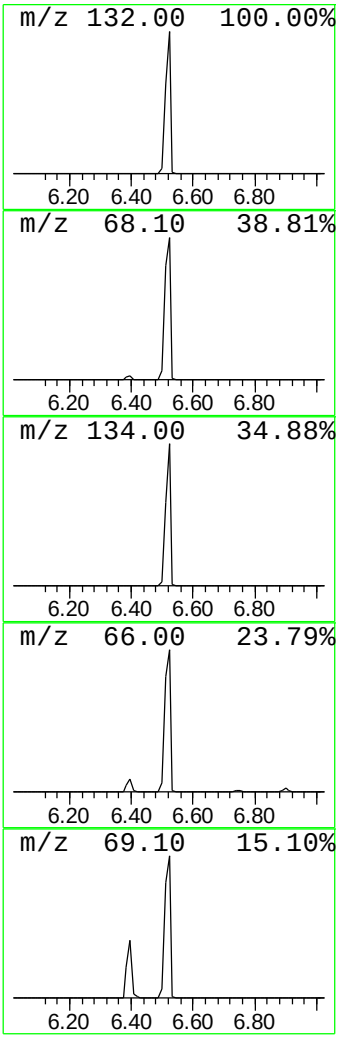
****

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	80.68 ng	6646630	1,4-Dichlorobenzene-d4	6.75

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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

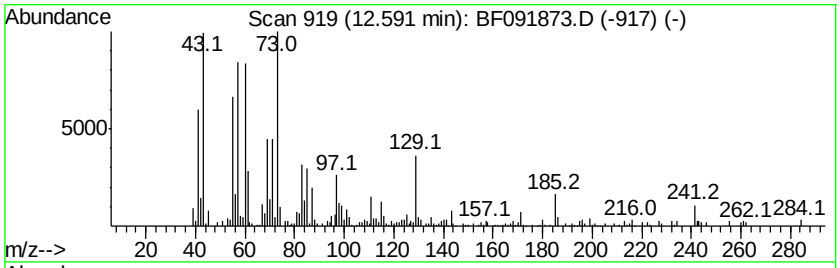
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

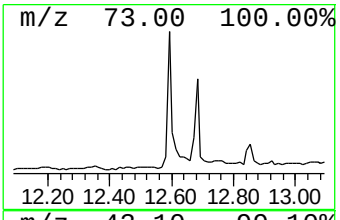
****

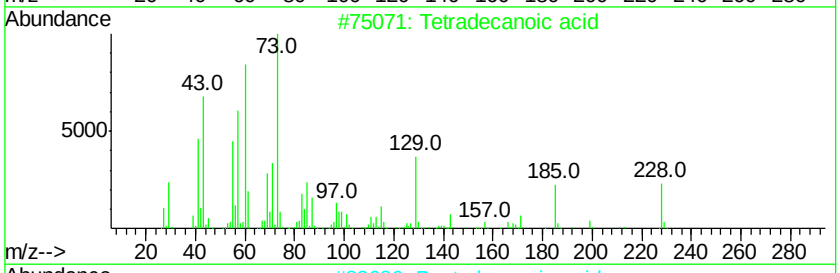
Peak Number 4 Tetradecanoic acid Concentration Rank 4

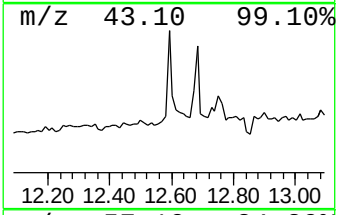
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.60 ng	278046	Chrysene-d12	13.89

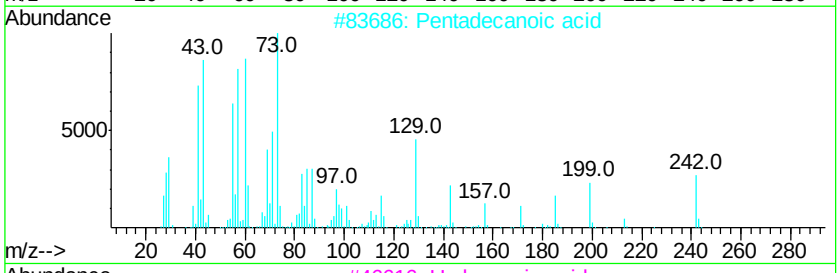
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	l-Tyrosinol	167	C9H13NO2	1000131-27-0	18

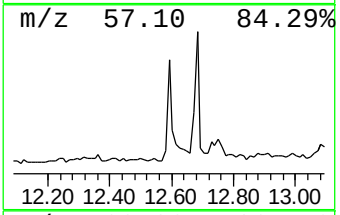


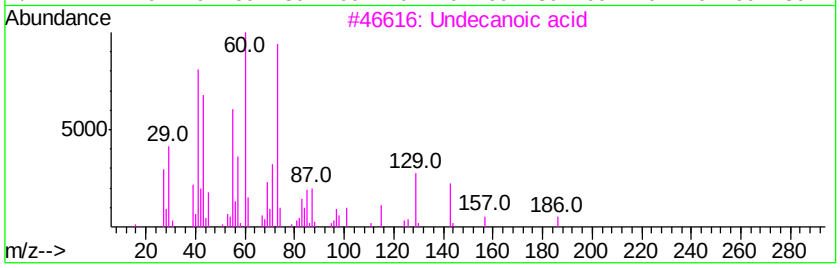


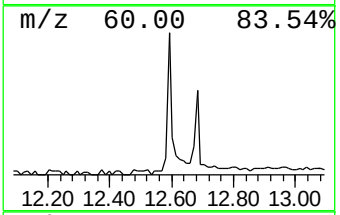


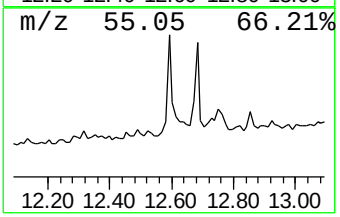












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122116\
Data File : BF091873.D
Acq On : 22 Dec 2016 9:22
Operator : UM/SJ
Sample : H6156-19
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.91	14.5	ng	1190810	1	6.75	1647580	20.0
unknown6.52	6.52	80.7	ng	6646630	1	6.75	1647580	20.0
Tetradecanoic acid	12.59	2.6	ng	278046	5	13.89	2137950	20.0