LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

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-BF012417.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	4.578	215	218	221	rBV	67990	90268	1.84%	0.249%
2	4.681	223	227	232	rVB	60257	87693	1.79%	0.242%
3	5.150	265	268	270	rBV	443939	637511	12.99%	1.759%
4	5.550	301	303	306	rVB	1716577	2375189	48.42%	6.552%
5	5.733	316	319	322	rBV	47326	51861	1.06%	0.143%
6	5.836	322	328	329	rBV3	22296	51987	1.06%	0.143%
7	5.973	338	340	344	rBV3	37148	82179	1.68%	0.227%
8	6.121	351	353	355	rBV2	55026	62540	1.27%	0.173%
9	6.579	390	393	395	rBV	1826029	1552039	31.64%	4.281%
10	6.727	403	406	408	rBV	3515206	3459780	70.52%	9.544%
11	6.922	418	423	425	rBV2	54519	111959	2.28%	0.309%
12	6.967	425	427	429	rBV	988617	974276	19.86%	2.687%
13	7.127	438	441	443	rVB	2752626	3303053	67.33%	9.111%
14	7.299	453	456	460	rVB4	37313	99342	2.02%	0.274%
15	7.367	460	462	464	rBV	53693	69661	1.42%	0.192%
16	7.482	468	472	473	rBV3	23795	59099	1.20%	0.163%
17	7.527	473	476	479	rVV	2330255	2827104	57.63%	7.798%
18	7.619	482	484	486	rBV2	80957	96664	1.97%	0.267%
19	7.996	514	517	519	rBV3	43522	83799	1.71%	0.231%
20	8.065	521	523	527	rBV3	47264	82788	1.69%	0.228%
21	8.259	537	540	542	rBV	1371976	1369584	27.92%	3.778%
22	8.625	569	572	579	rBV5	51326	97477	1.99%	0.269%
23	9.345	632	635	637	rBV	4253388	4905869	100.00%	13.532%
24	9.733	666	669	671	rVB	250702	218465	4.45%	0.603%
25	10.019	691	694	696	rBV	1594453	1436204	29.28%	3.962%
26	10.808	760	763	766	rBV	2489905	2701398	55.06%	7.452%
27	10.922	771	773	778	rVB2	41540	65738	1.34%	0.181%
28	11.379	811	813	819	rBV2	57261	87797	1.79%	0.242%
29	11.505	822	824	826	rBV	1630993	1404346	28.63%	3.874%
30	12.031	868	870	877	rBV	76429	104128	2.12%	0.287%
31	13.094	960	963	966	rBV	3382336	4814202	98.13%	13.280%
32	13.985	1039	1041	1046	rBV	114834	164113	3.35%	0.453%
33	14.145	1052	1055	1057	rBV	1564088	1493145	30.44%	4.119%
34	15.620	1181	1184	1187	rBV	952088	1231412	25.10%	3.397%

LSC Area Percent Report

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Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 36252670

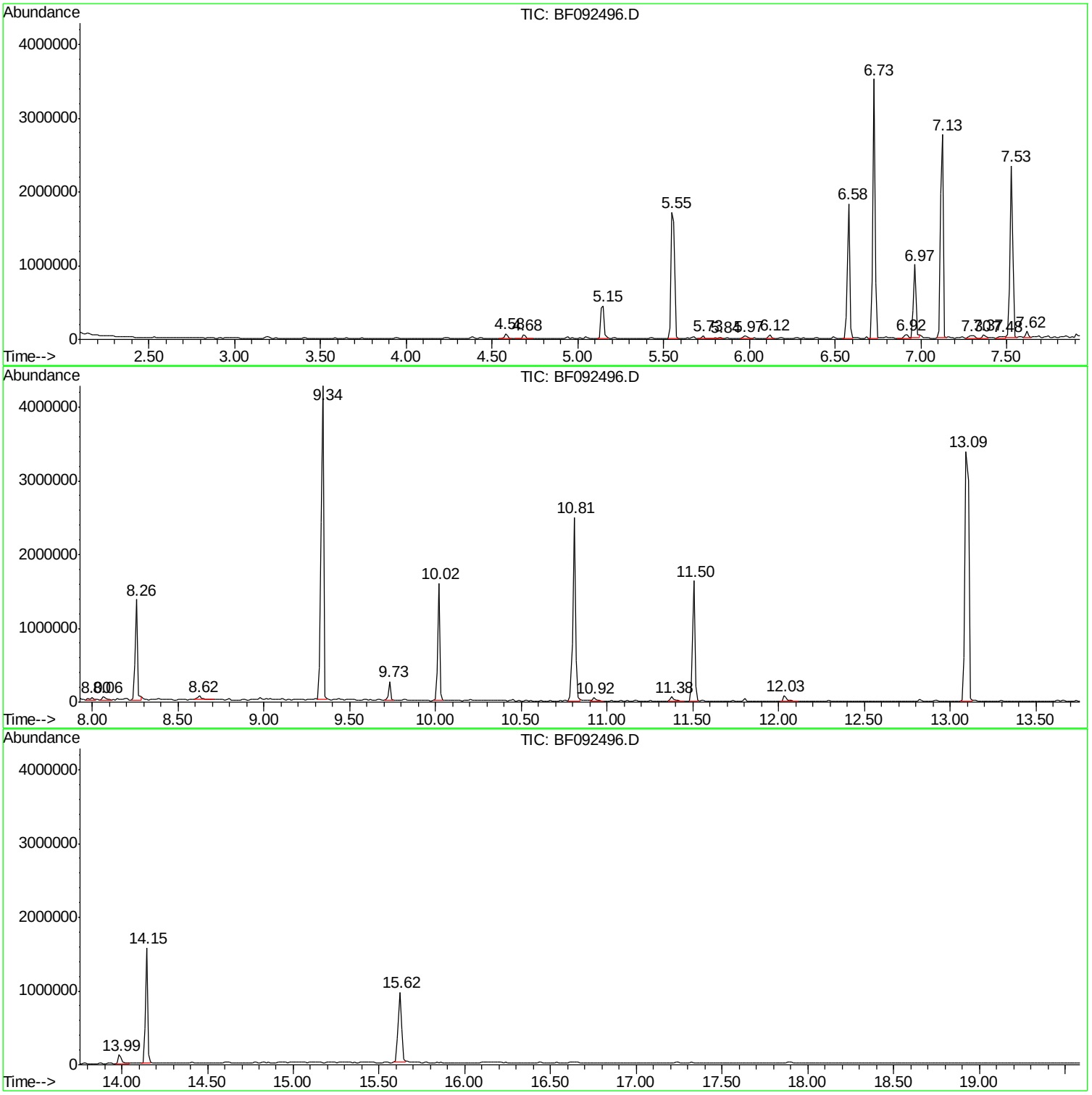
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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\BF012517\
Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

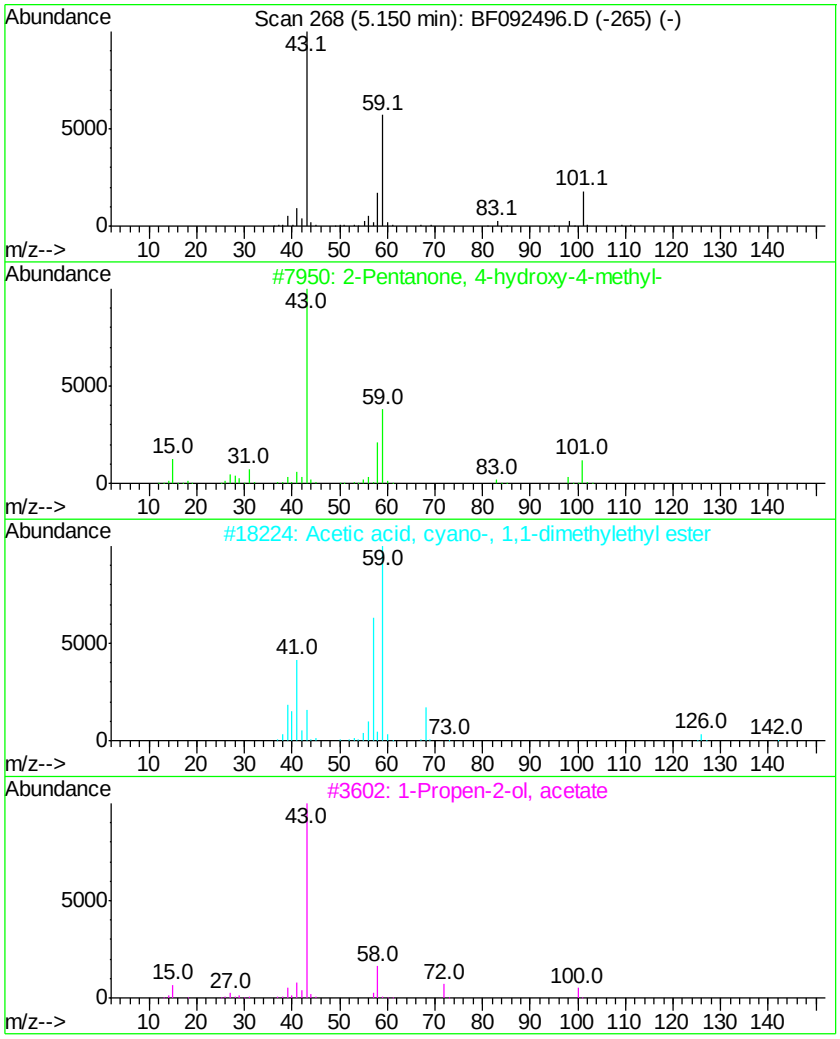
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

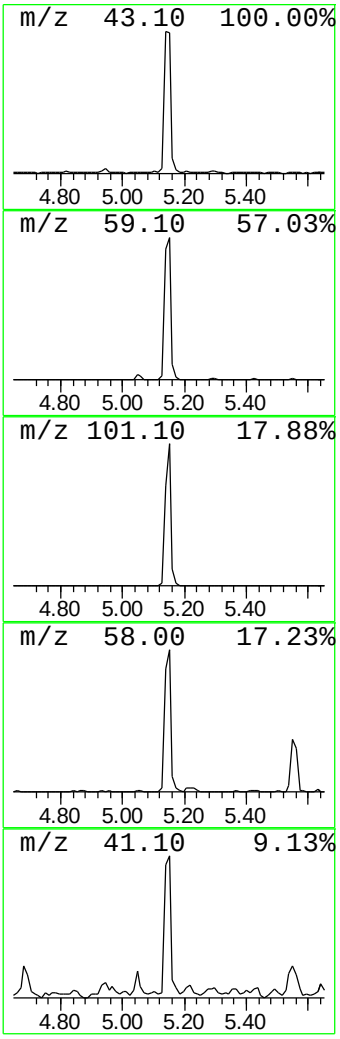
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.09 ng	637511	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

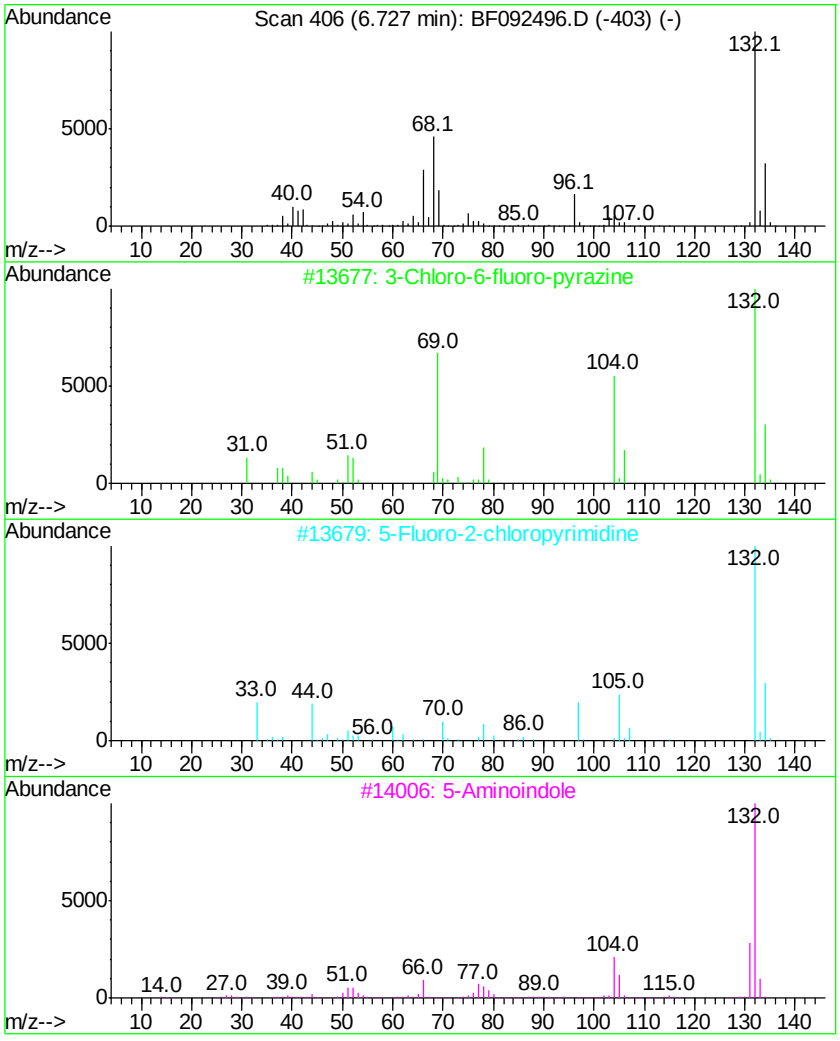
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

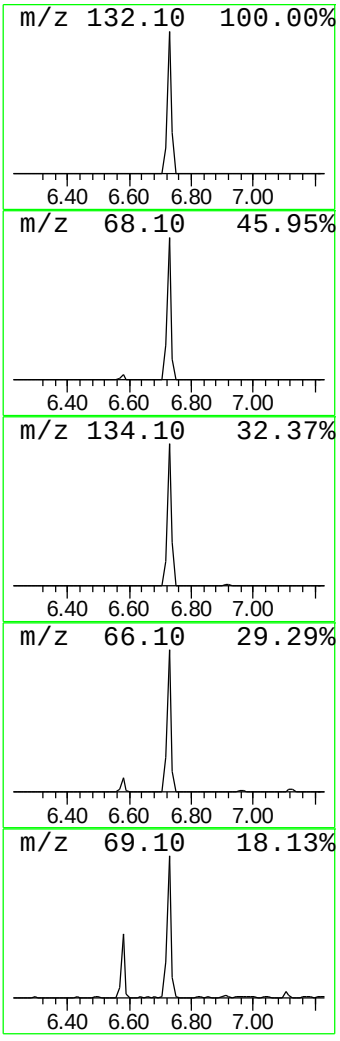
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	71.02 ng	3459780	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092496.D
Acq On : 26 Jan 2017 00:14
Operator : SJ/MA
Sample : I1398-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PMW-2-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

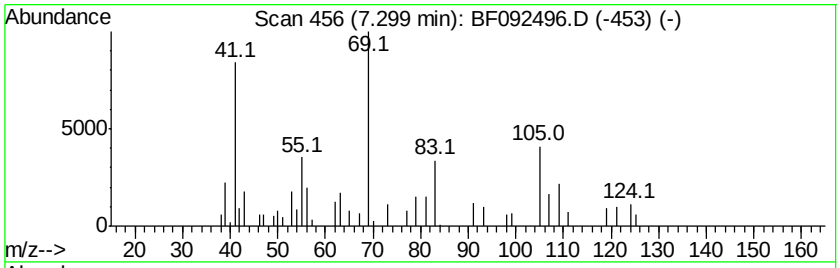
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

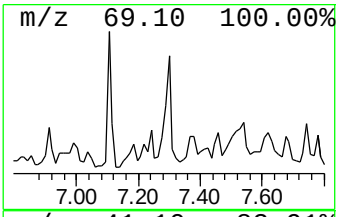
****

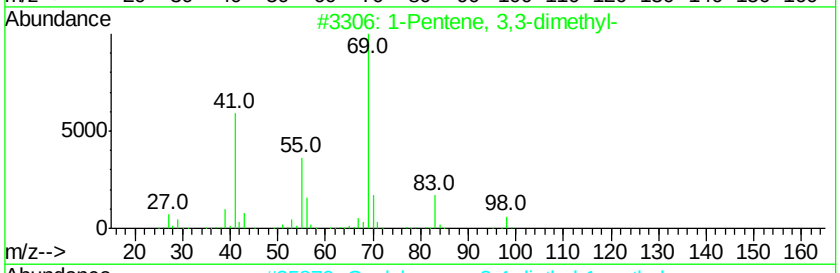
Peak Number 4 unknown7.30 Concentration Rank 5

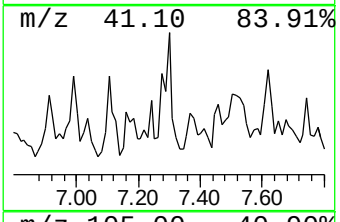
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	2.04 ng	99342	1,4-Dichlorobenzene-d4	6.97

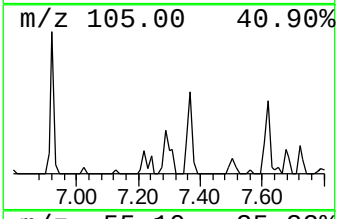
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	35
2	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	17
3	Imidazole, 4-trifluoromethyl-5-n...	181	C4H2F3N3O2	104752-68-3	10
4	3-Butyn-2-ol, 2-methyl-	84	C5H8O	000115-19-5	10
5	Butane, 1,3-dichloro-2-methyl-	140	C5H10Cl2	023010-07-3	10

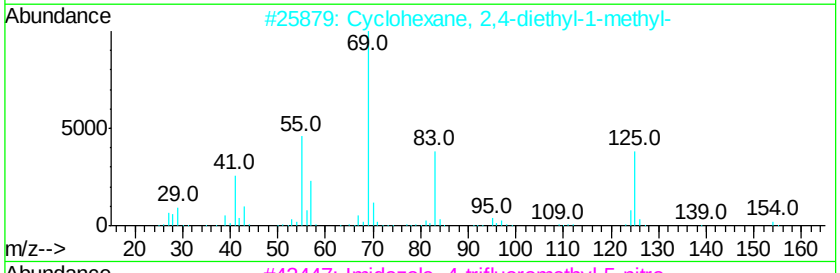


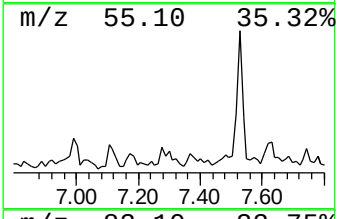


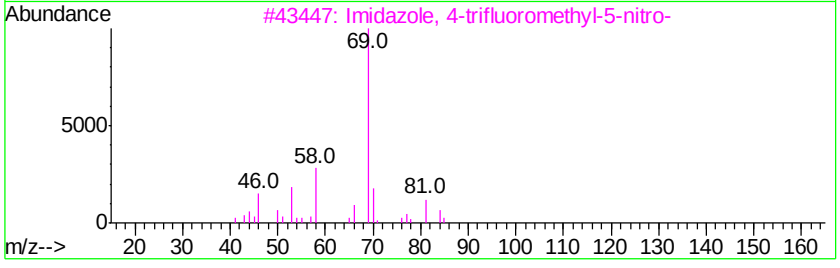


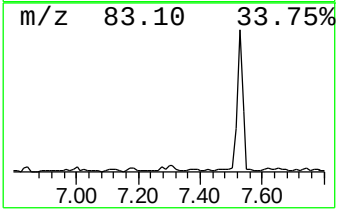












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

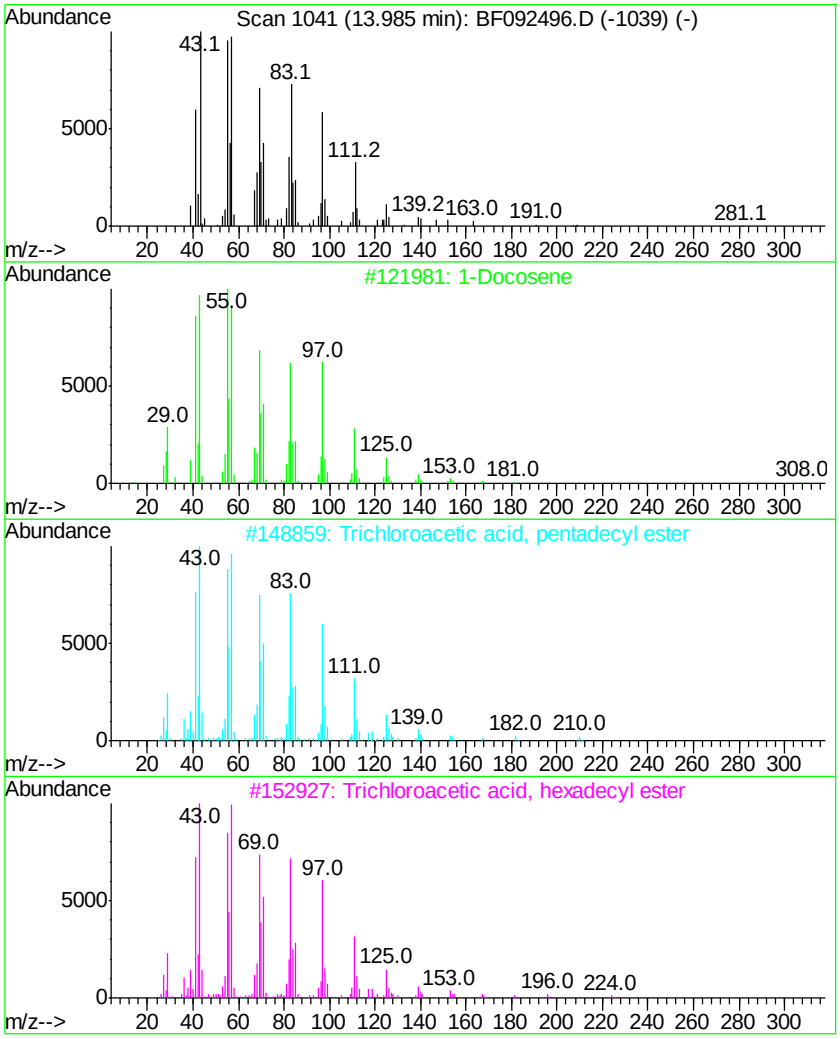
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

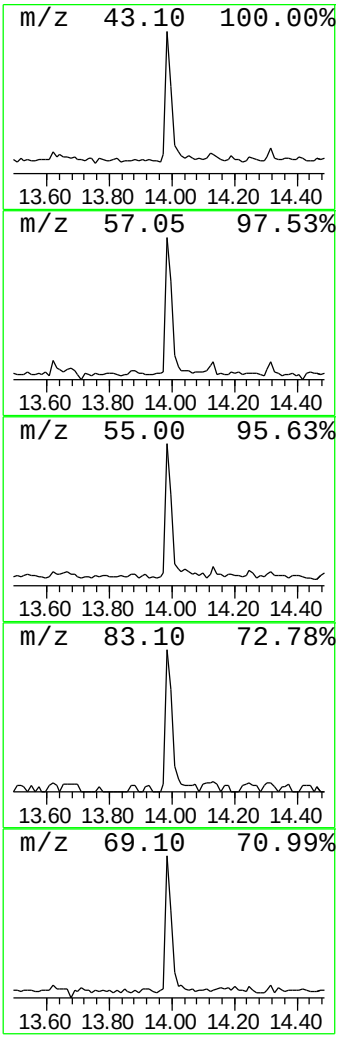
****

Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	2.20 ng	164113	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	1-Nonadecanol	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

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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...	5.15	13.1	ng	637511	1	6.97	974276	20.0
unknown6.73	6.73	71.0	ng	3459780	1	6.97	974276	20.0
unknown7.30	7.30	2.0	ng	99342	1	6.97	974276	20.0
1-Docosene	13.99	2.2	ng	164113	5	14.15	1493150	20.0