LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109780.D
Acq On : 11 Oct 2018 9:30
Operator : JU/SJ
Sample : J5299-09
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-M

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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	4.875	471	474	487	rBV	60585	79132	2.49%	0.454%
2	5.310	545	548	567	rBV	381553	597145	18.80%	3.430%
3	6.345	720	724	741	rBV	200739	439643	13.84%	2.525%
4	6.463	741	744	769	rVV	1176382	1467567	46.20%	8.429%
5	6.692	780	783	804	rBV	366175	514009	16.18%	2.952%
6	6.851	806	810	839	rVB	2046091	2059173	64.83%	11.826%
7	7.263	875	880	913	rBV	1246006	1781153	56.07%	10.230%
8	7.975	997	1001	1024	rBV	512103	659834	20.77%	3.790%
9	9.051	1180	1184	1212	rBV	2990833	3176422	100.00%	18.243%
10	9.445	1248	1251	1258	rBV	50423	54895	1.73%	0.315%
11	9.722	1294	1298	1319	rBV	692544	733768	23.10%	4.214%
12	10.510	1428	1432	1450	rBV	868978	1108065	34.88%	6.364%
13	11.198	1546	1549	1575	rBV	521944	679333	21.39%	3.902%
14	12.610	1786	1789	1795	rBV	131706	115449	3.63%	0.663%
15	12.780	1814	1818	1833	rBV	2387196	2539996	79.96%	14.588%
16	13.310	1905	1908	1912	rBV	99436	81973	2.58%	0.471%
17	13.827	1992	1996	2010	rBV	501533	574393	18.08%	3.299%
18	14.592	2123	2126	2132	rVB	44979	41867	1.32%	0.240%
19	14.904	2175	2179	2184	rBV	45867	45798	1.44%	0.263%
20	15.227	2229	2234	2247	rBV	360158	572798	18.03%	3.290%
21	15.645	2299	2305	2310	rBV	36464	52105	1.64%	0.299%
22	16.104	2377	2383	2388	rBV3	22504	37309	1.17%	0.214%

Sum of corrected areas: 17411827

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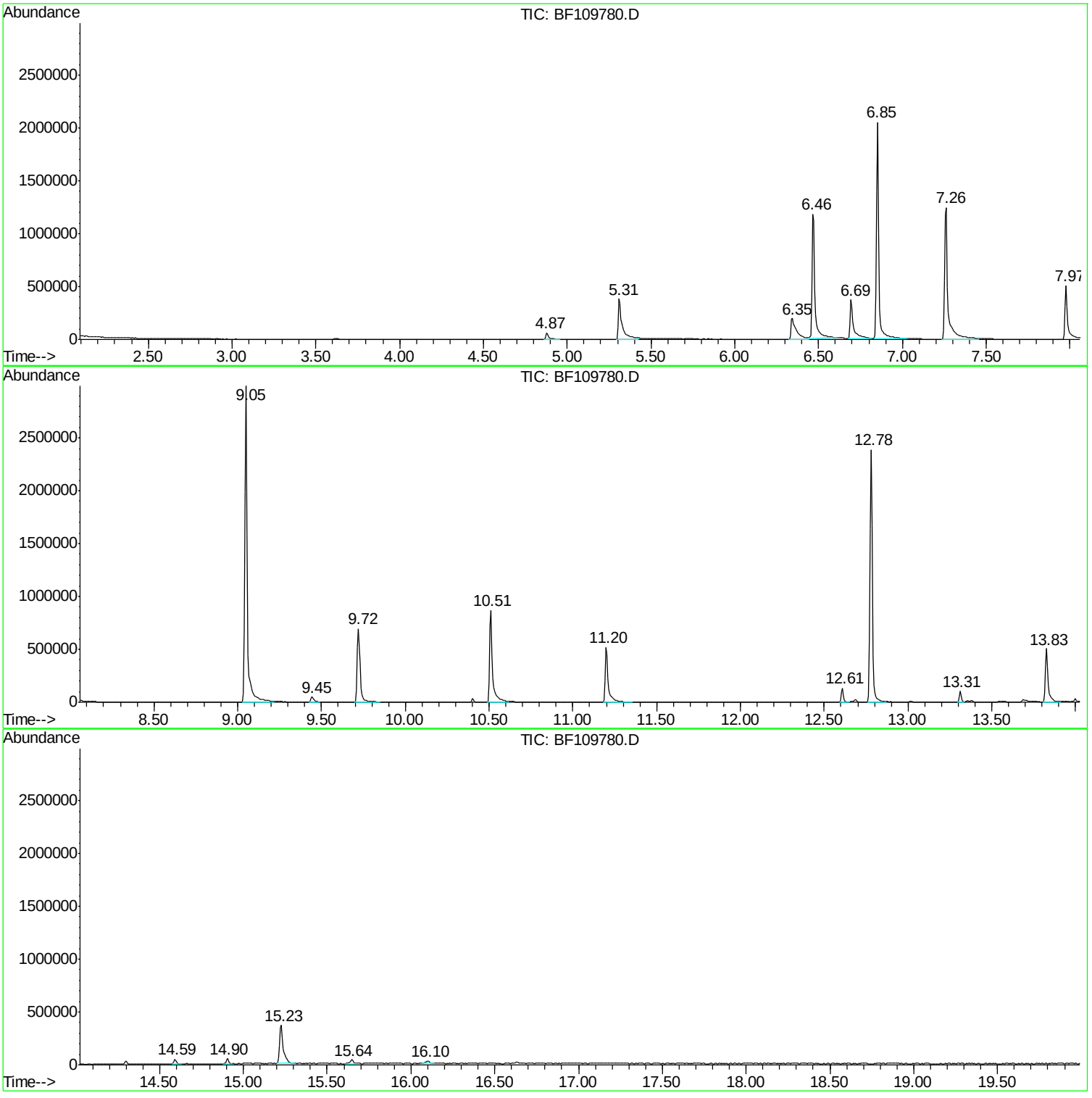
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100518-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109780.D
Acq On : 11 Oct 2018 9:30
Operator : JU/SJ
Sample : J5299-09
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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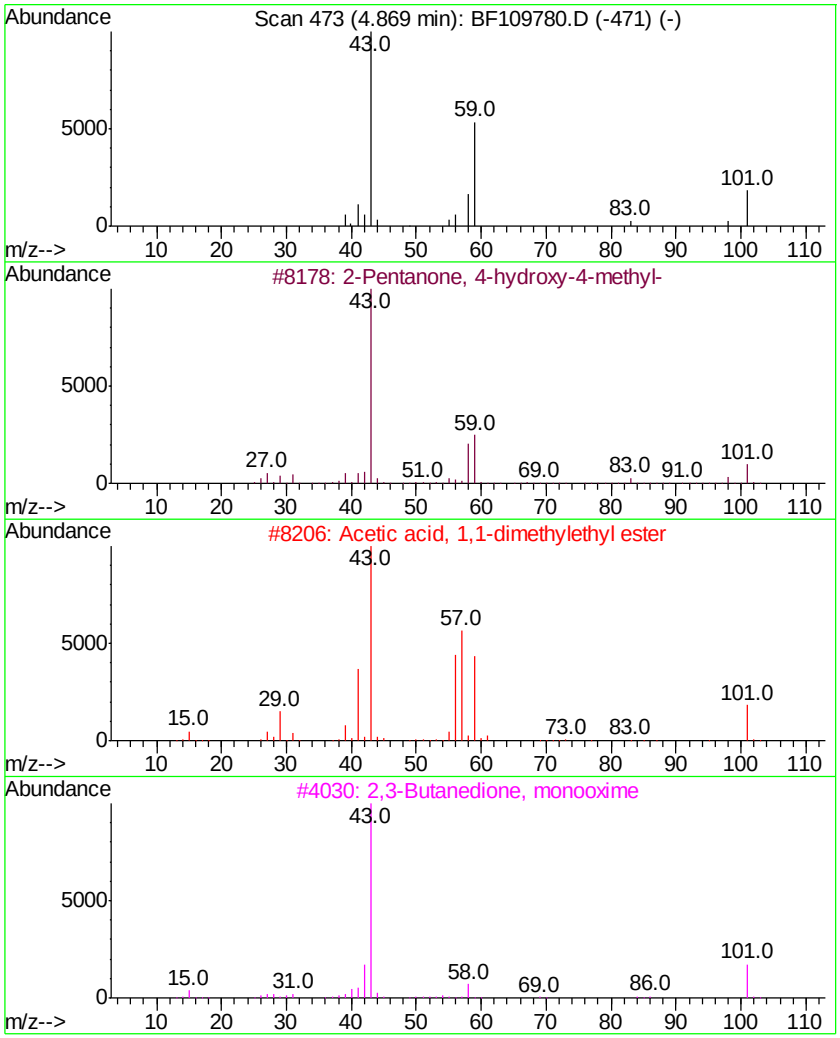
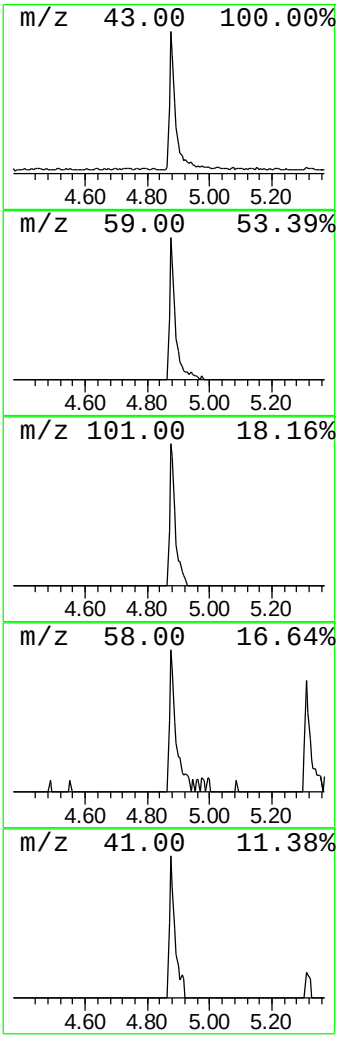
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	3.08 ng	79132	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109780.D
Acq On : 11 Oct 2018 9:30
Operator : JU/SJ
Sample : J5299-09
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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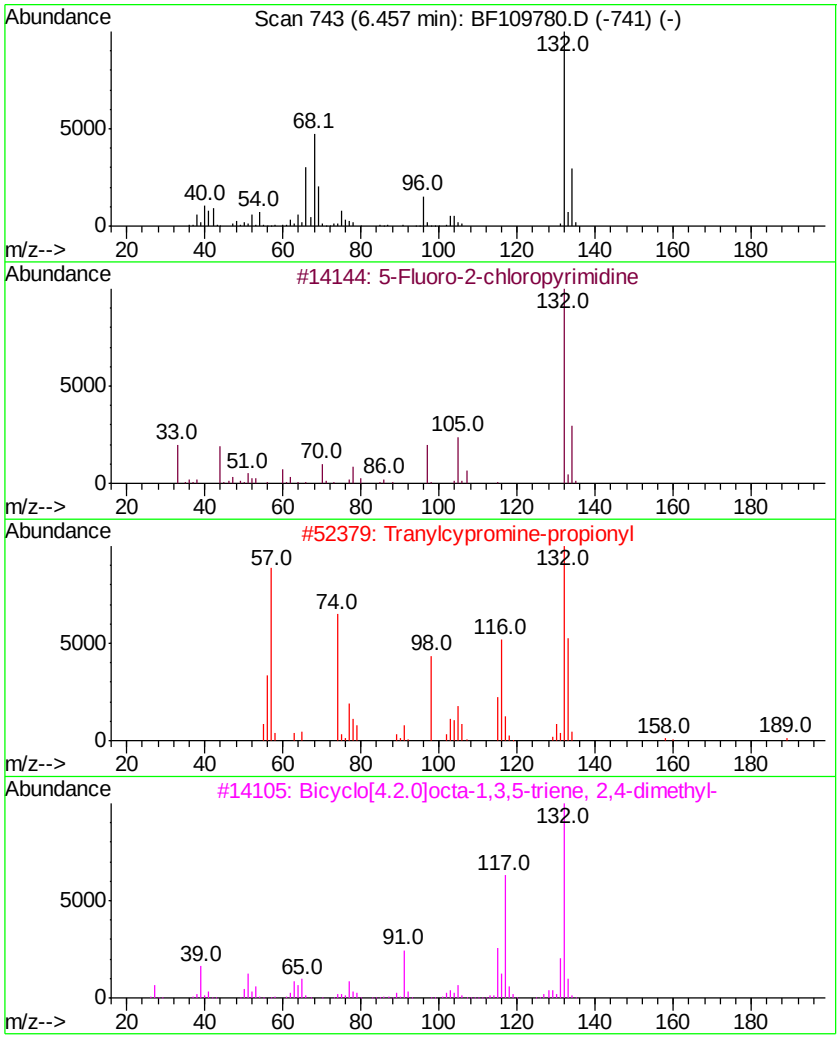
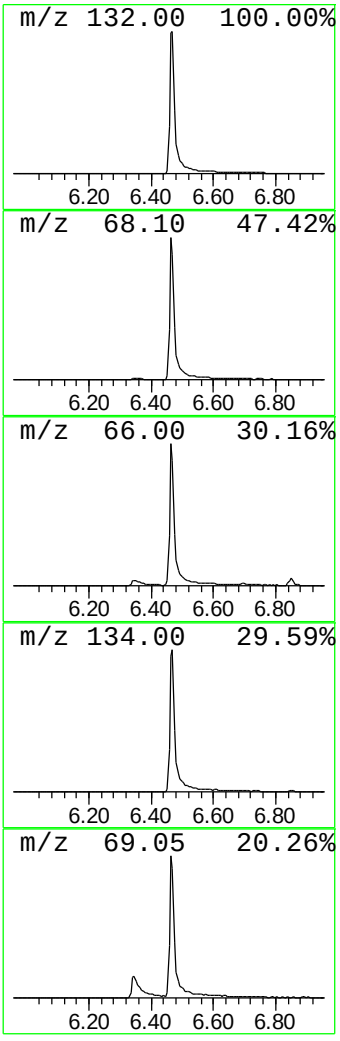
Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	57.10 ng	1467570	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF109780.D
Acq On : 11 Oct 2018 9:30
Operator : JU/SJ
Sample : J5299-09
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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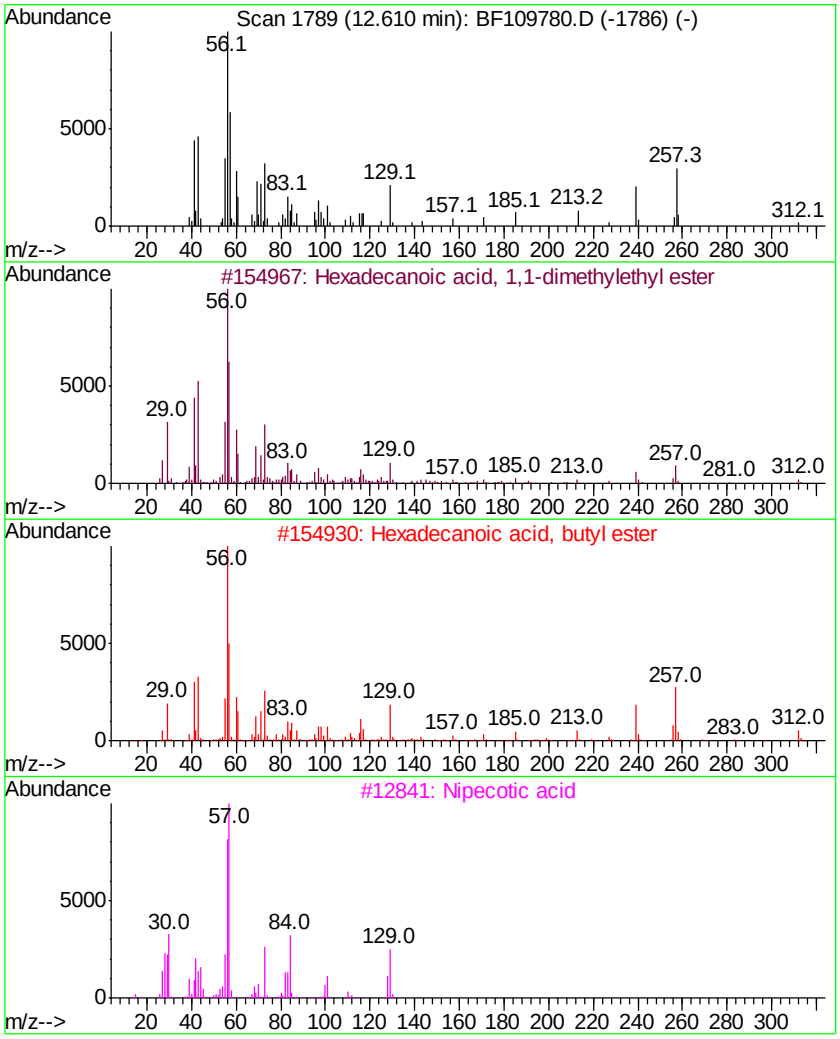
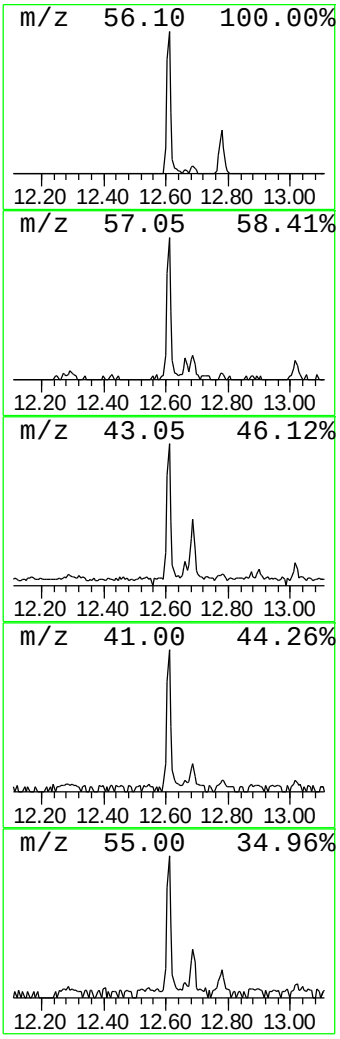
Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	4.02 ng	115449	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30





Library Search Compound Report

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Data File : BF109780.D
Acq On : 11 Oct 2018 9:30
Operator : JU/SJ
Sample : J5299-09
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

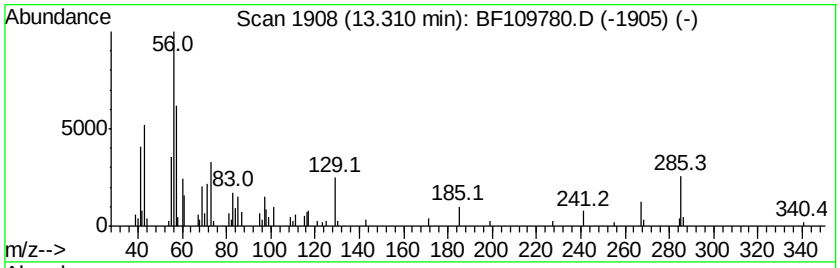
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

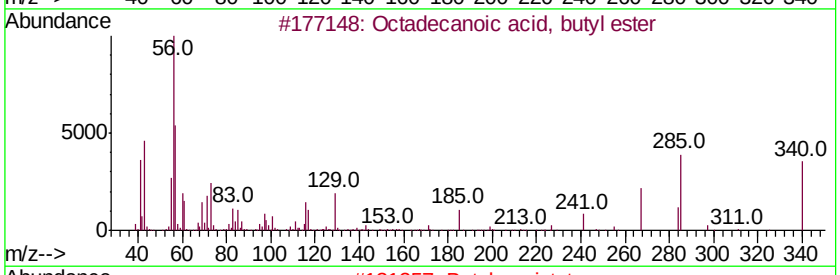
****

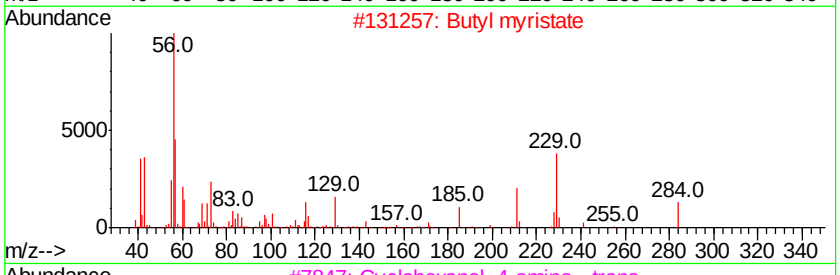
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

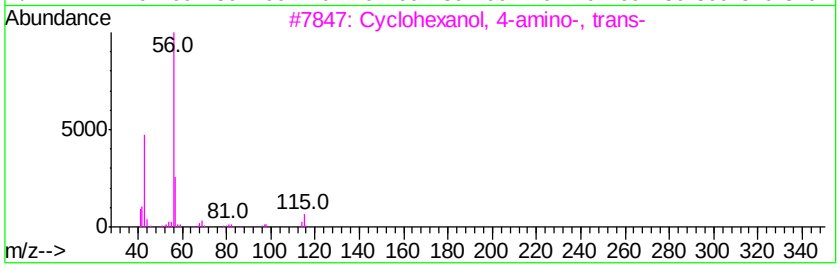
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	2.85 ng	81973	Chrysene-d12	13.83

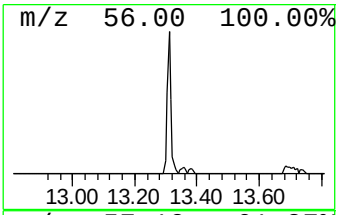
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	Butyl myristate	284	C18H36O2	000110-36-1	59
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27

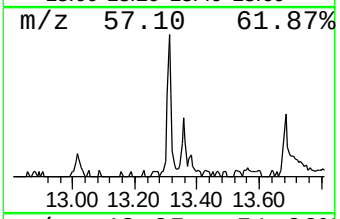


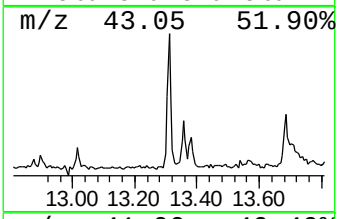


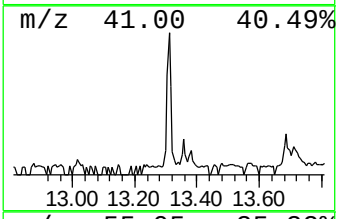


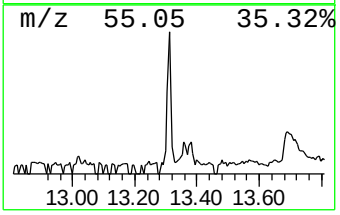












Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.87	3.1	ng	79132	1	6.69	514009	20.0
unknown6.46	6.46	57.1	ng	1467570	1	6.69	514009	20.0
Hexadecanoic acid...	12.61	4.0	ng	115449	5	13.83	574393	20.0
Octadecanoic acid...	13.31	2.9	ng	81973	5	13.83	574393	20.0