LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109778.D
Acq On : 11 Oct 2018 8:34
Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-D-S

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	484	rBV	62911	79527	2.49%	0.445%
2	5.310	545	548	564	rBV	376714	577652	18.10%	3.231%
3	6.345	720	724	741	rBV	209733	436861	13.68%	2.444%
4	6.463	741	744	767	rVV	1139031	1445143	45.27%	8.083%
5	6.692	780	783	806	rBV	387812	525555	16.46%	2.940%
6	6.851	806	810	836	rBV	2031522	2039604	63.89%	11.408%
7	7.257	875	879	913	rBV	1186578	1783385	55.87%	9.975%
8	7.975	997	1001	1036	rBV	546187	702584	22.01%	3.930%
9	9.051	1180	1184	1229	rBV	2946281	3192263	100.00%	17.855%
10	9.445	1248	1251	1260	rBV	61766	68719	2.15%	0.384%
11	9.722	1294	1298	1315	rBV	730553	749481	23.48%	4.192%
12	10.510	1428	1432	1451	rBV	831069	1103146	34.56%	6.170%
13	11.198	1546	1549	1572	rBV	517969	698782	21.89%	3.909%
14	12.610	1786	1789	1792	rBV	96806	77841	2.44%	0.435%
15	12.780	1814	1818	1833	rBV	2562586	2714367	85.03%	15.182%
16	13.310	1905	1908	1912	rBV	66472	54678	1.71%	0.306%
17	13.686	1968	1972	1988	rBV4	29241	78208	2.45%	0.437%
18	13.827	1992	1996	2009	rVV	585566	659074	20.65%	3.686%
19	14.298	2074	2076	2082	rVB	34617	33267	1.04%	0.186%
20	14.592	2123	2126	2131	rVB	55153	49675	1.56%	0.278%
21	14.904	2175	2179	2185	rVB	58571	62007	1.94%	0.347%
22	15.227	2229	2234	2245	rBV	394246	636415	19.94%	3.560%
23	15.645	2300	2305	2312	rVB	43215	58199	1.82%	0.326%
24	16.104	2377	2383	2388	rBV2	30891	52008	1.63%	0.291%

Sum of corrected areas: 17878441

LSC Report - Integrated Chromatogram

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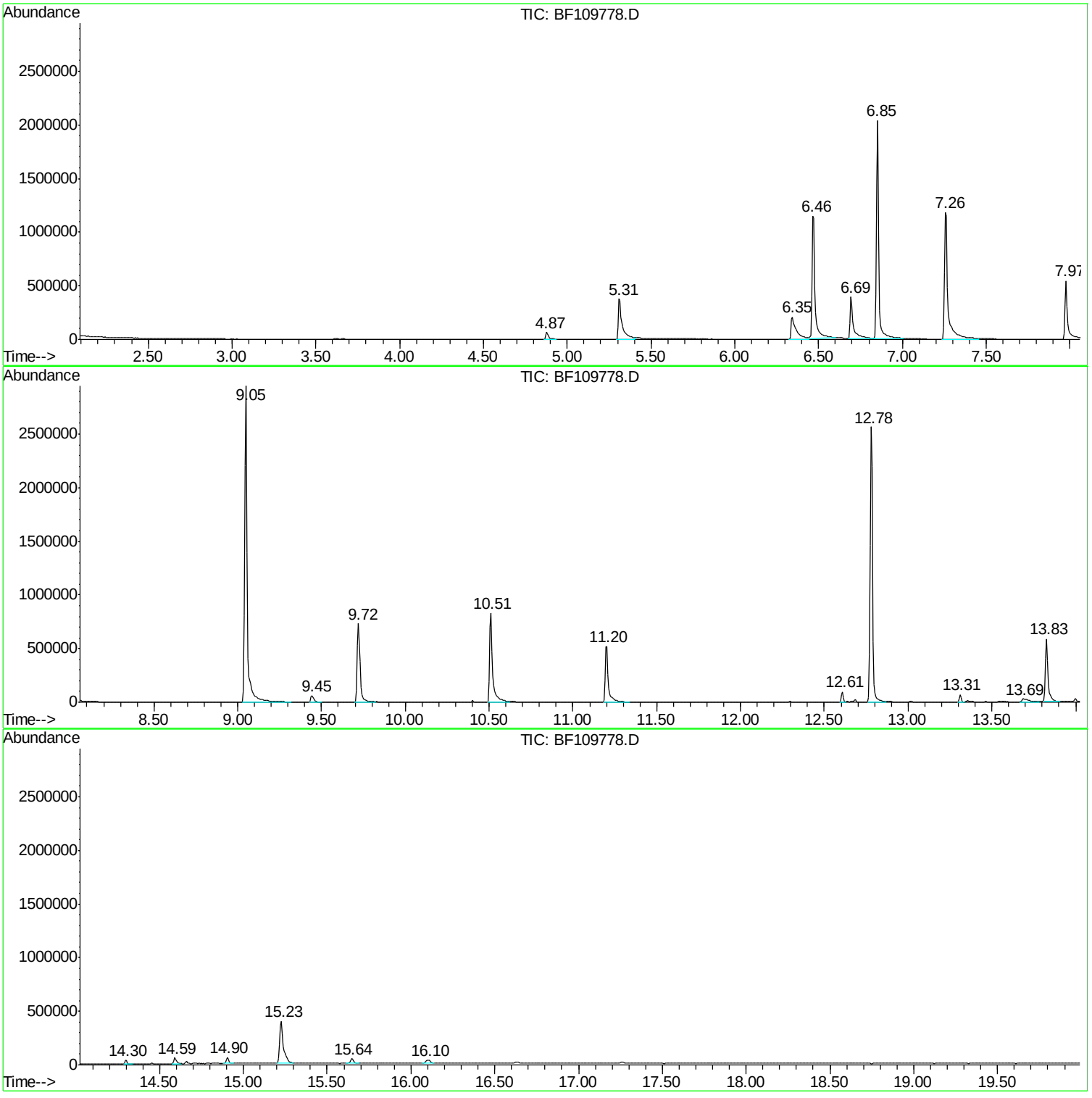
Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100518-SIDI-F-D-S

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109778.D
Acq On : 11 Oct 2018 8:34
Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-D-S

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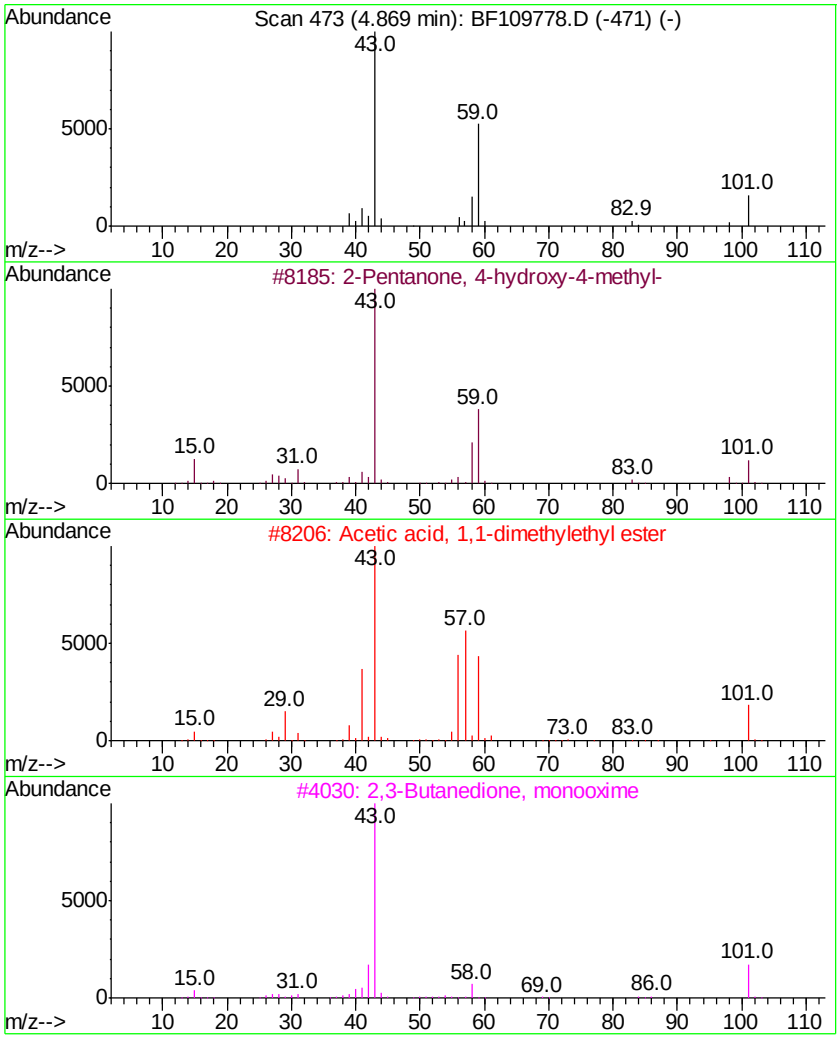
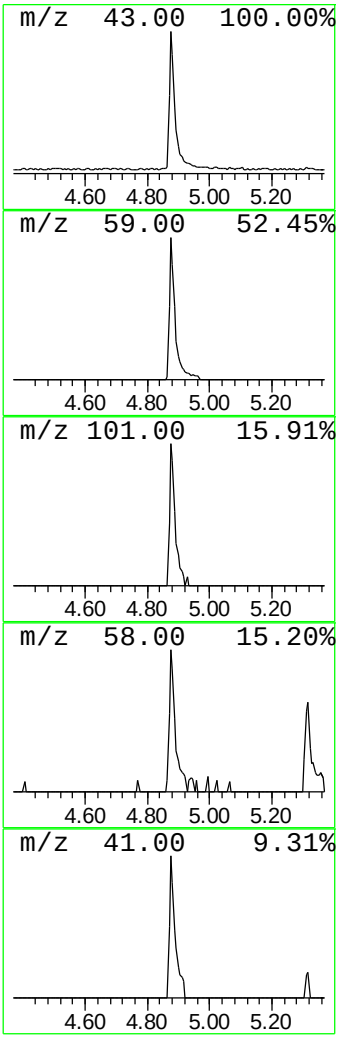
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	3.03 ng	79527	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	40
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	3-Heptanol	116	C7H16O	000589-82-2	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
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Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-D-S

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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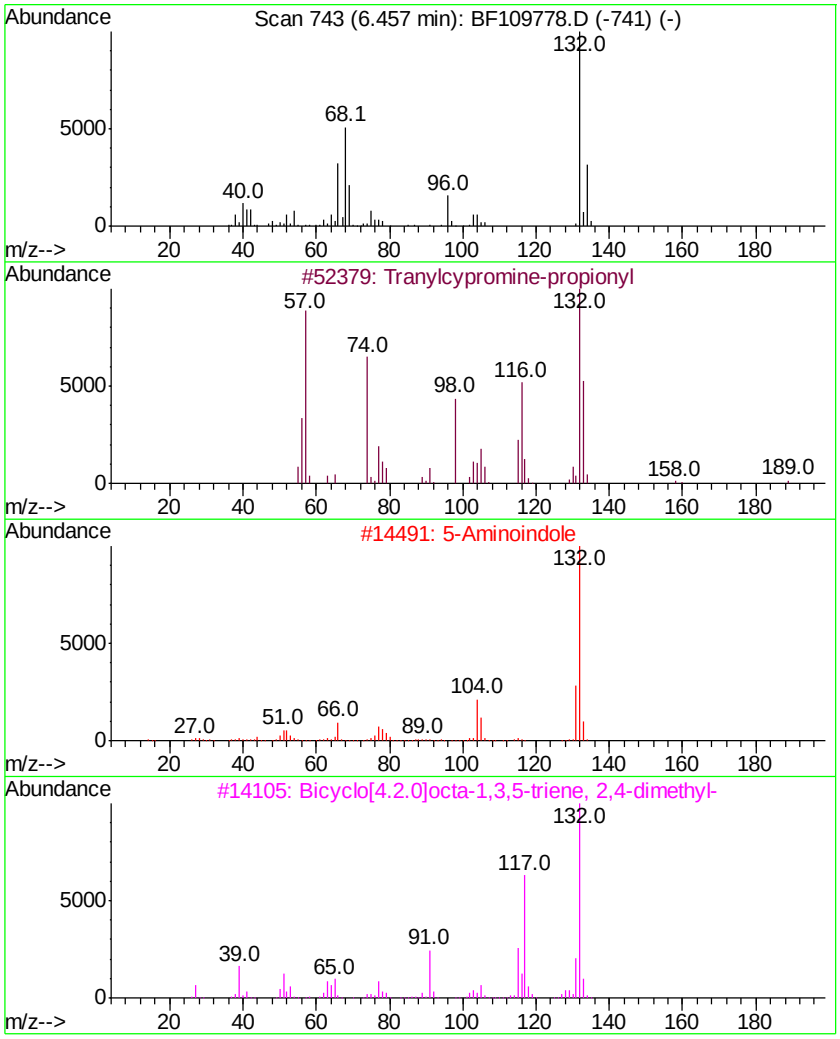
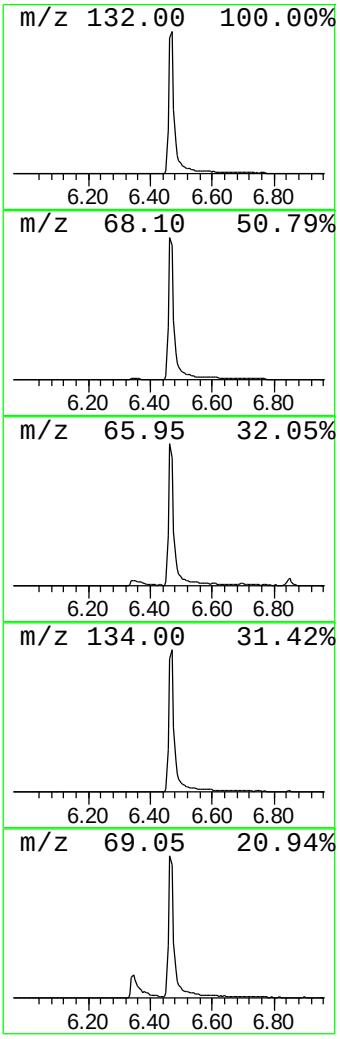
Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	54.99 ng	1445140	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2	5-Aminoindole	132	C8H8N2	005192-03-0	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF109778.D
Acq On : 11 Oct 2018 8:34
Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-D-S

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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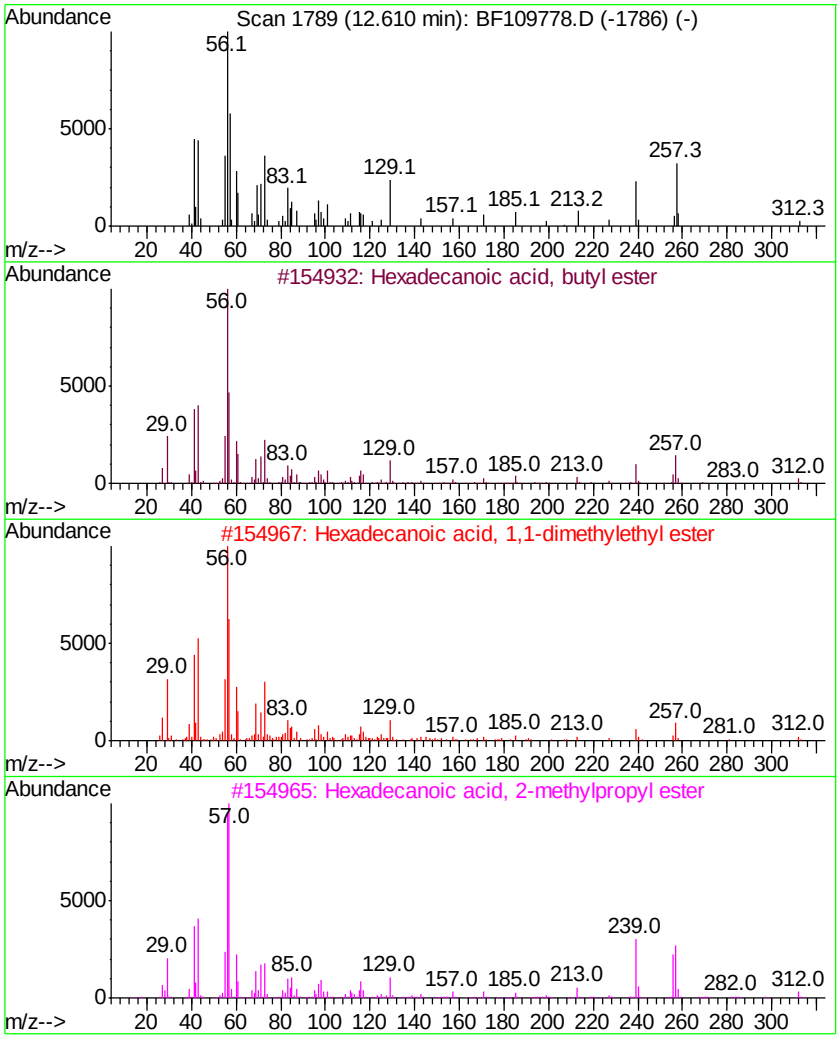
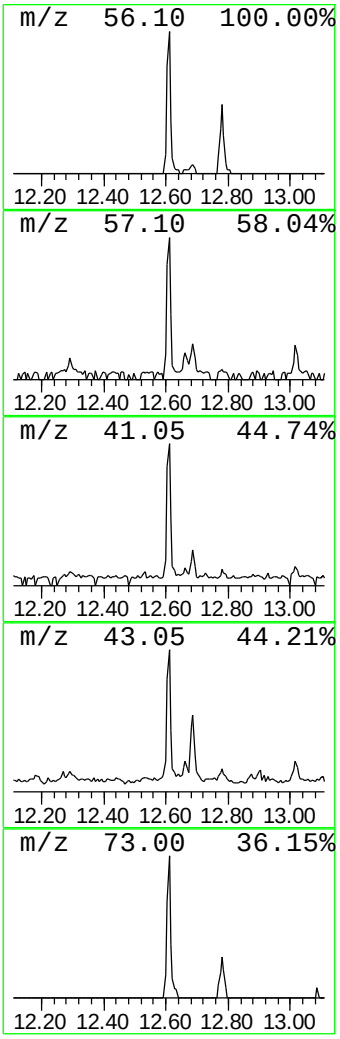
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	2.36 ng	77841	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	68
4	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	43
5	Nipecotic acid	129	C6H11NO2	000498-95-3	38





Library Search Compound Report

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Data File : BF109778.D
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Operator : JU/SJ
Sample : J5299-07
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-D-S

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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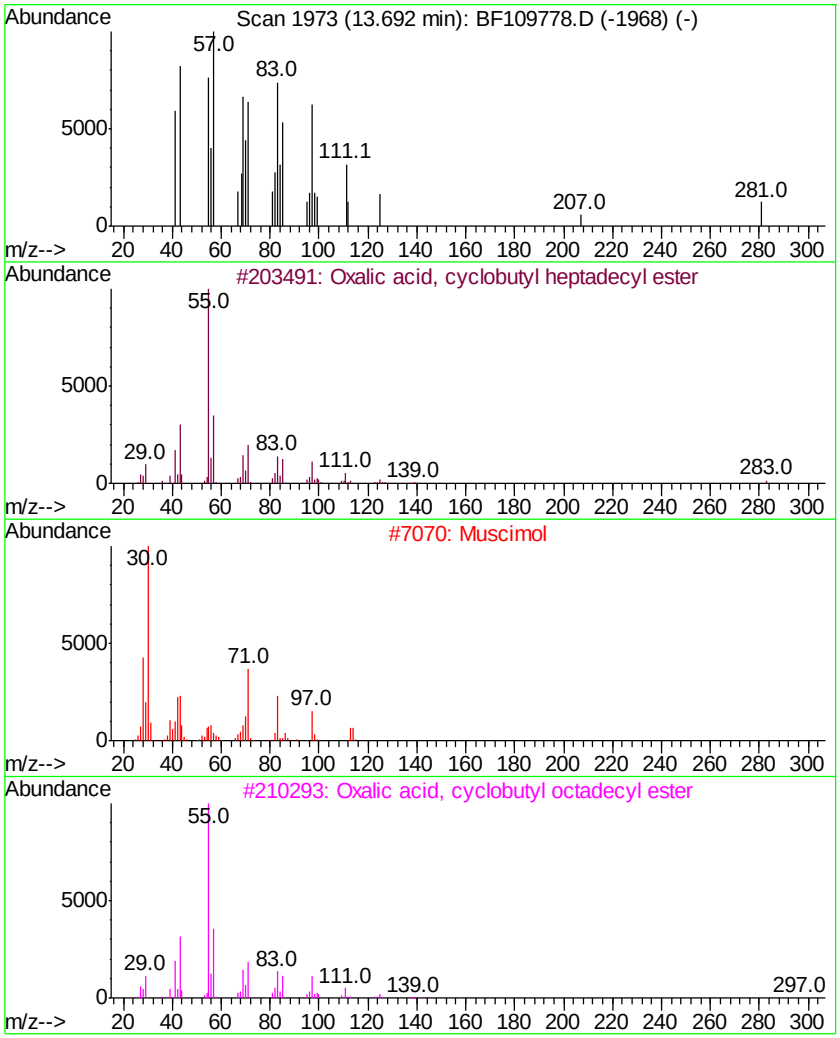
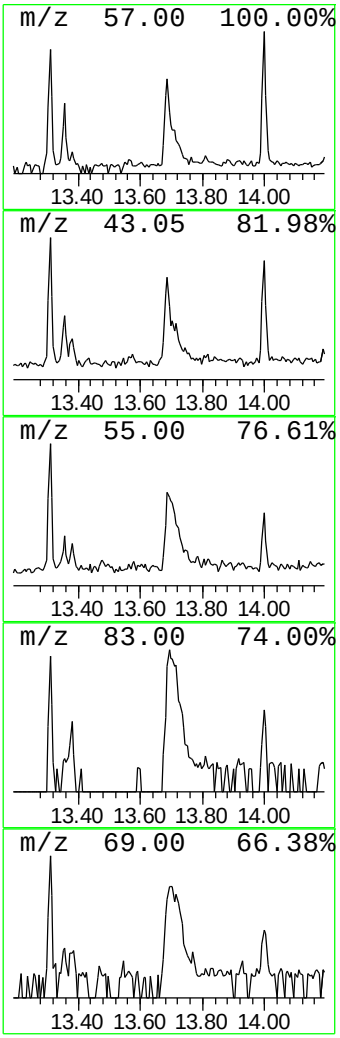
Peak Number 5 Oxalic acid, cyclobutyl hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	2.37 ng	78208	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	50
2	Muscimol	114	C4H6N2O2	002763-96-4	50
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	50
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	47
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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	3.0	ng	79527	1	6.69	525555	20.0
unknown6.46	6.46	55.0	ng	1445140	1	6.69	525555	20.0
Hexadecanoic acid...	12.61	2.4	ng	77841	5	13.83	659074	20.0
Oxalic acid, cycl...	13.69	2.4	ng	78208	5	13.83	659074	20.0