LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112460.D
Acq On : 8 Feb 2019 15:30
Operator : JU/SJ
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08(0-2)

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-BF012519.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	2.134	3	8	17	rVB	157668	230022	5.82%	0.693%
2	3.916	306	311	319	rVB	42481	60197	1.52%	0.181%
3	5.063	503	506	519	rVB	117095	183247	4.64%	0.552%
4	5.428	564	568	569	rBV	42706	44320	1.12%	0.134%
5	5.475	572	576	597	rVB	3540052	3550944	89.86%	10.705%
6	6.487	743	748	765	rBV	3501166	3846983	97.35%	11.598%
7	6.610	765	769	772	rVV	4315155	3951776	100.00%	11.914%
8	6.657	774	777	782	rVB	69568	72628	1.84%	0.219%
9	6.828	803	806	814	rBV	858270	837944	21.20%	2.526%
10	6.987	829	833	837	rBV	3114050	2917556	73.83%	8.796%
11	7.398	898	903	906	rBV	2459357	2305384	58.34%	6.950%
12	8.110	1019	1024	1037	rBV	1038016	1129813	28.59%	3.406%
13	9.186	1202	1207	1210	rBV	4262549	3800968	96.18%	11.459%
14	9.581	1270	1274	1282	rVB	288274	270845	6.85%	0.817%
15	9.869	1319	1323	1333	rVB	1299176	1194985	30.24%	3.603%
16	10.663	1454	1458	1467	rBV	2863468	2763644	69.93%	8.332%
17	11.357	1572	1576	1587	rBV	1259377	1207896	30.57%	3.642%
18	11.886	1662	1666	1673	rBV2	535646	641750	16.24%	1.935%
19	12.669	1796	1799	1805	rBV	374755	420595	10.64%	1.268%
20	12.939	1841	1845	1850	rBV	2951382	2717346	68.76%	8.192%
21	13.833	1995	1997	2002	rBV	310620	302479	7.65%	0.912%
22	14.010	2024	2027	2030	rBV	773076	718628	18.18%	2.167%

Sum of corrected areas: 33169950

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112460.D
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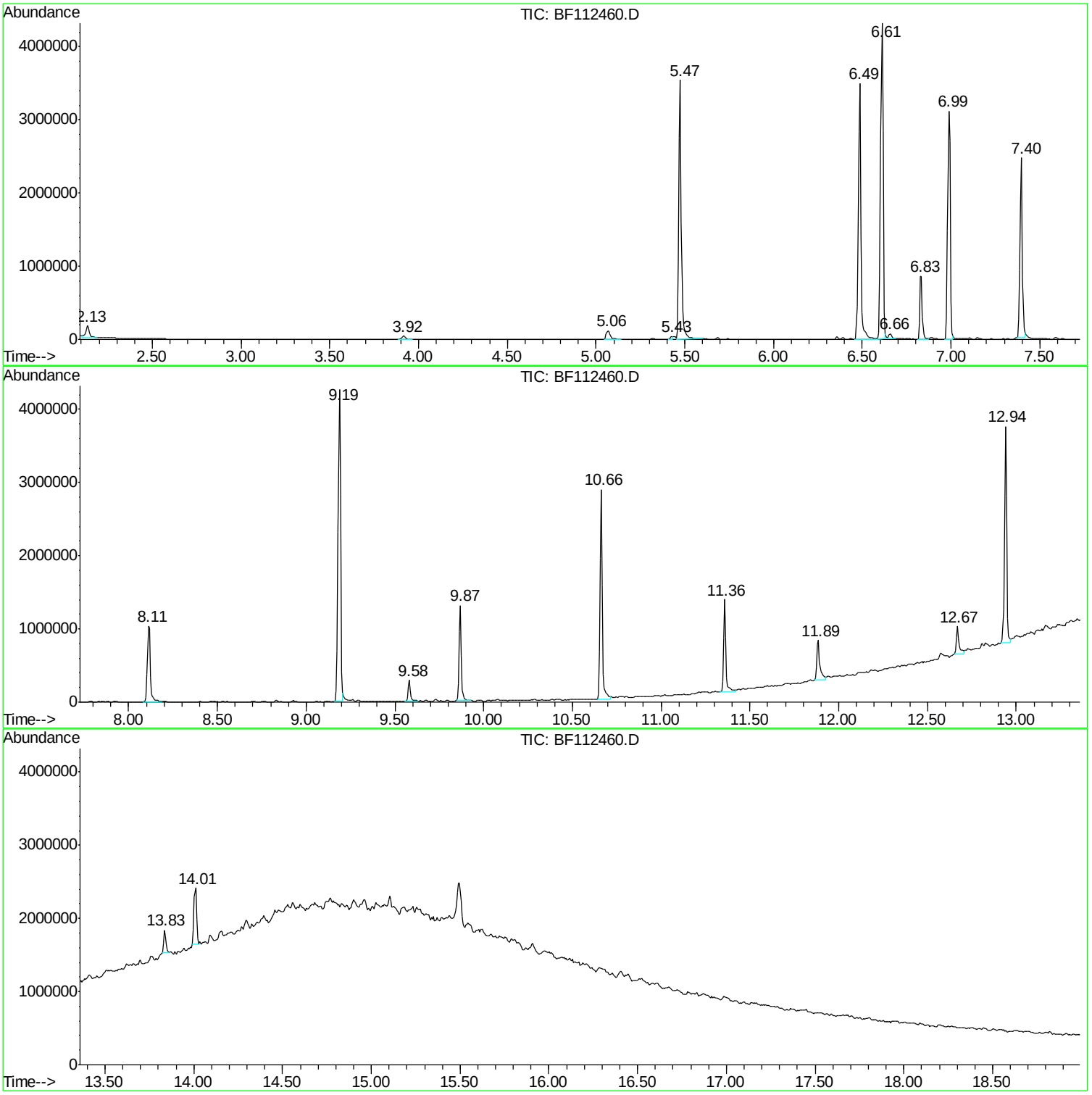
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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\BF020819\
Data File : BF112460.D
Acq On : 8 Feb 2019 15:30
Operator : JU/SJ
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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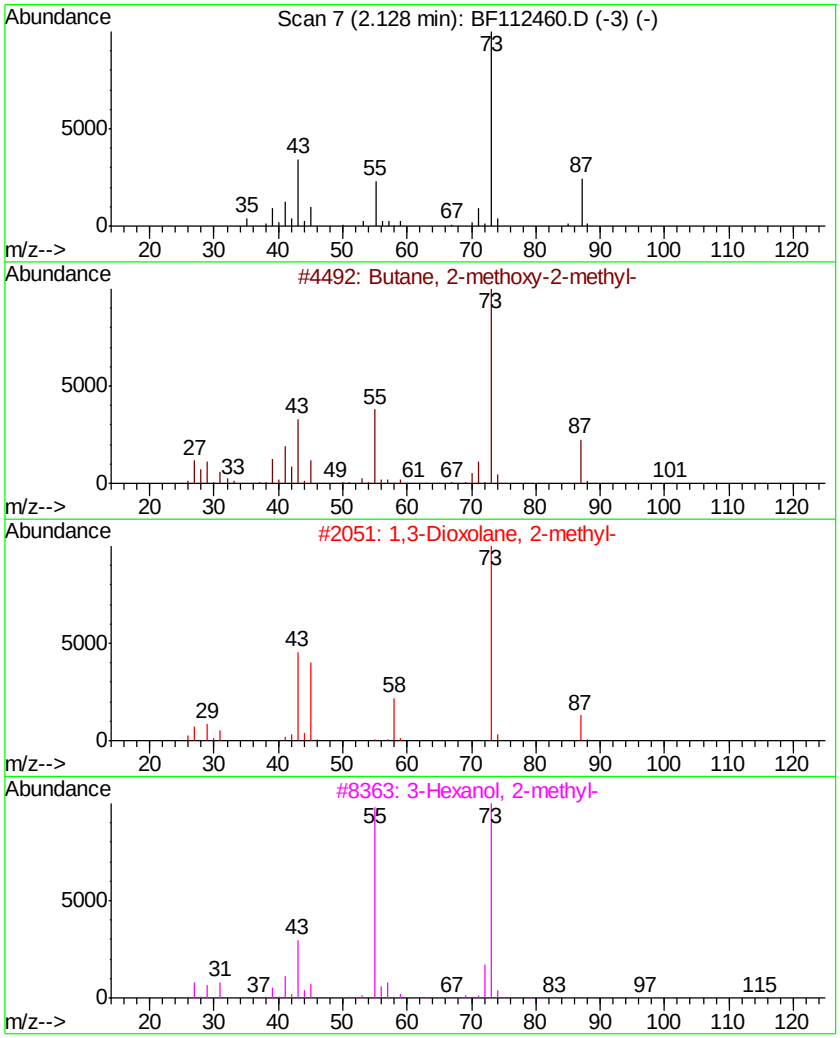
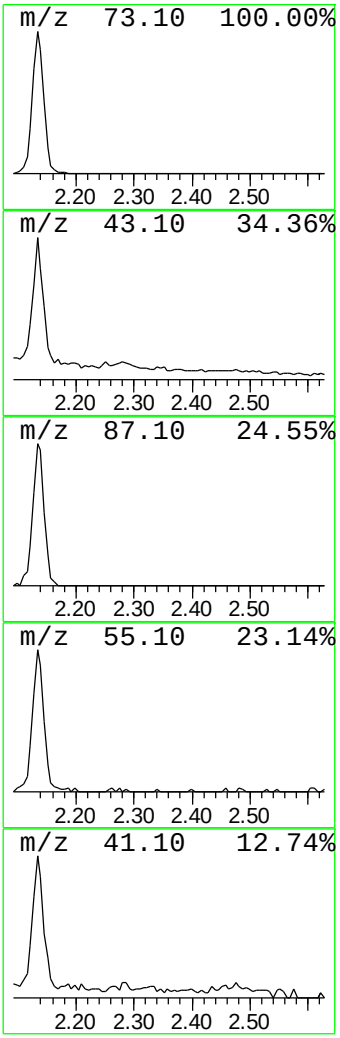
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	5.49 ng	230022	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-08(0-2)

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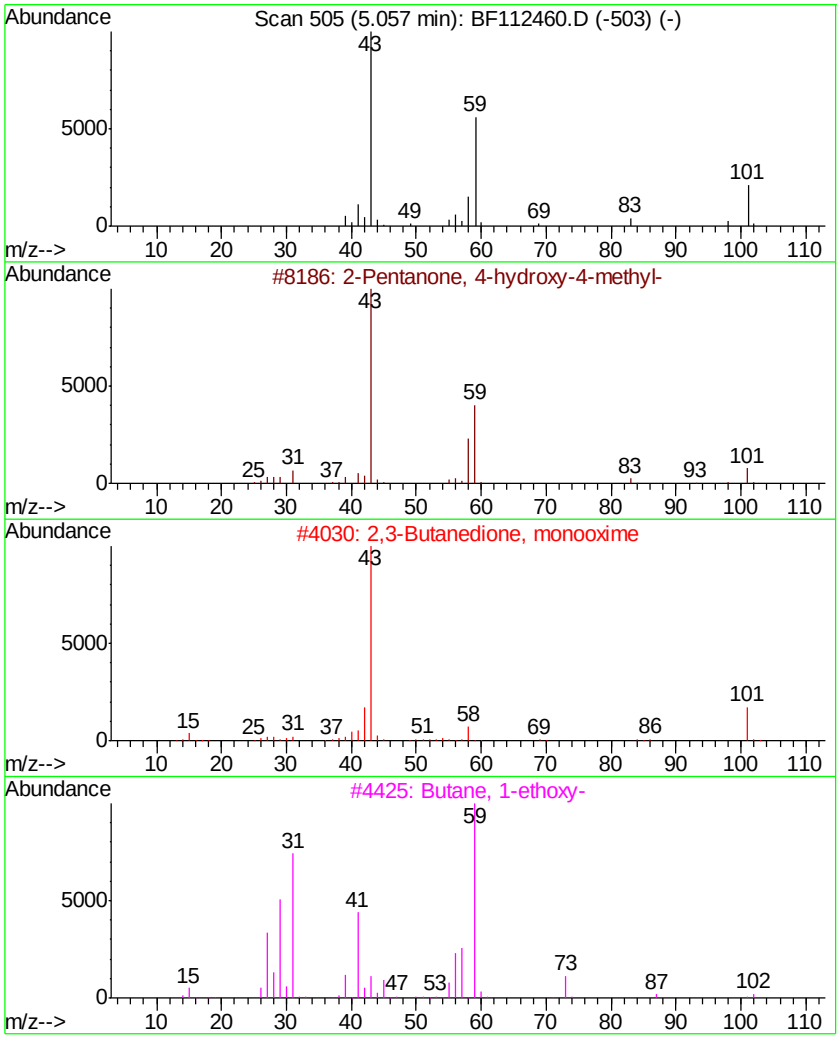
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

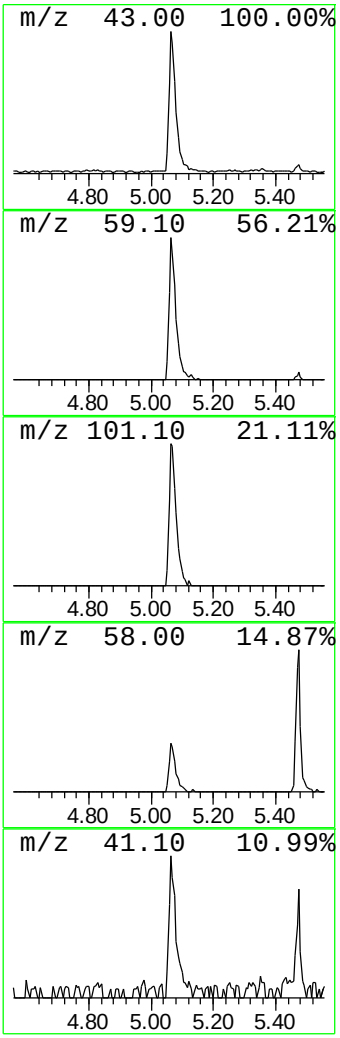
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	4.37 ng	183247	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
Data File : BF112460.D
Acq On : 8 Feb 2019 15:30
Operator : JU/SJ
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

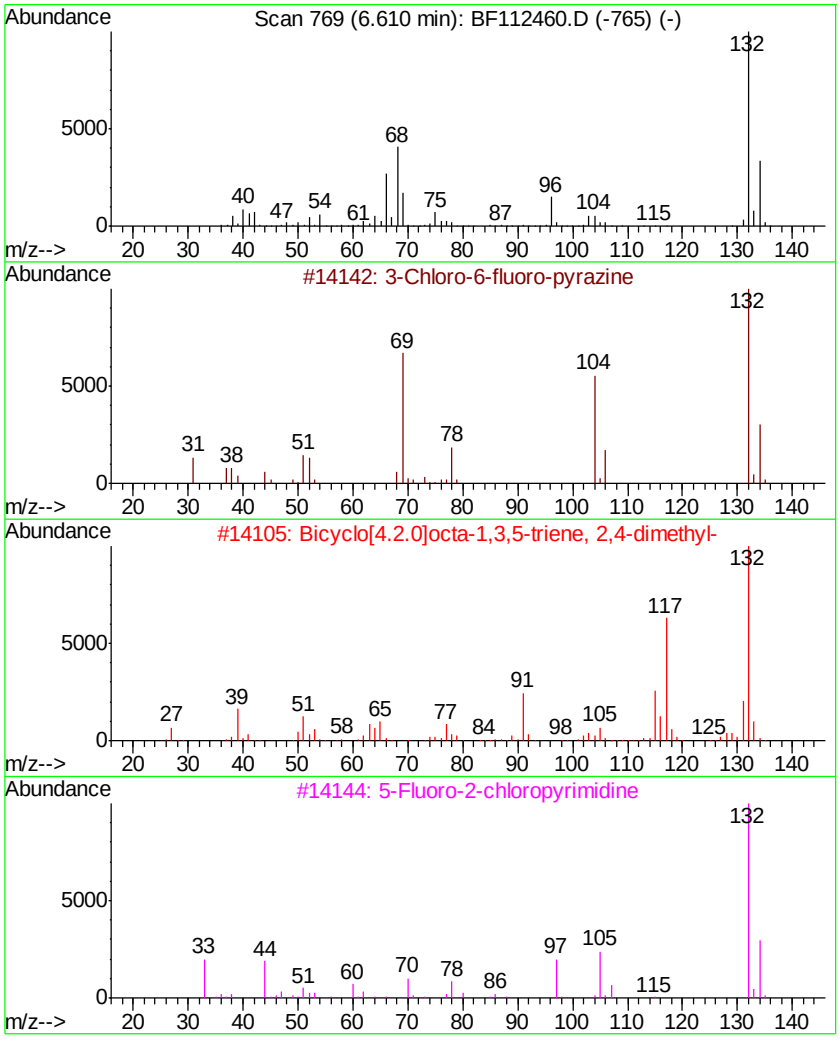
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

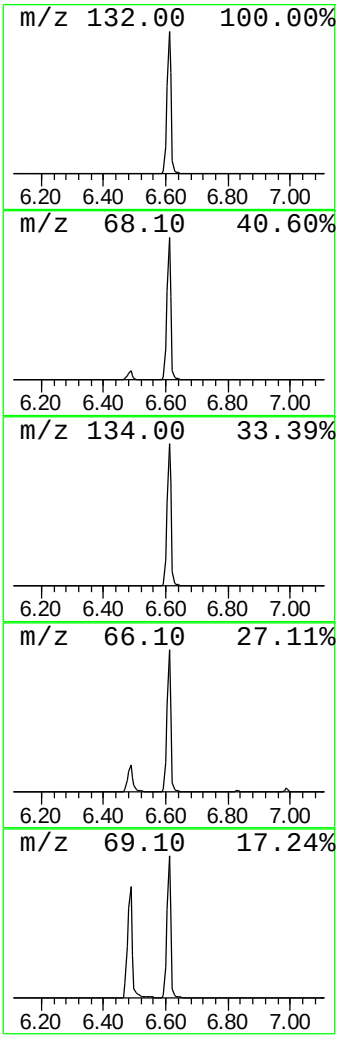
****

Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	94.32 ng	3951780	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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Data File : BF112460.D
Acq On : 8 Feb 2019 15:30
Operator : JU/SJ
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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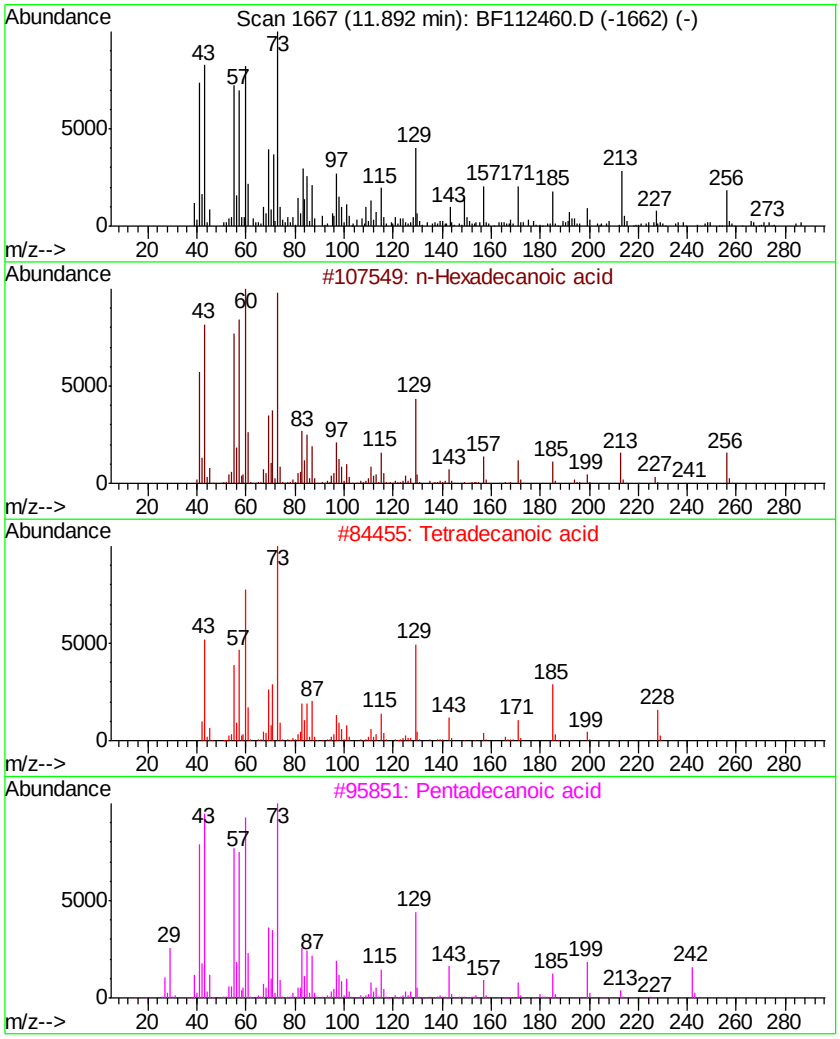
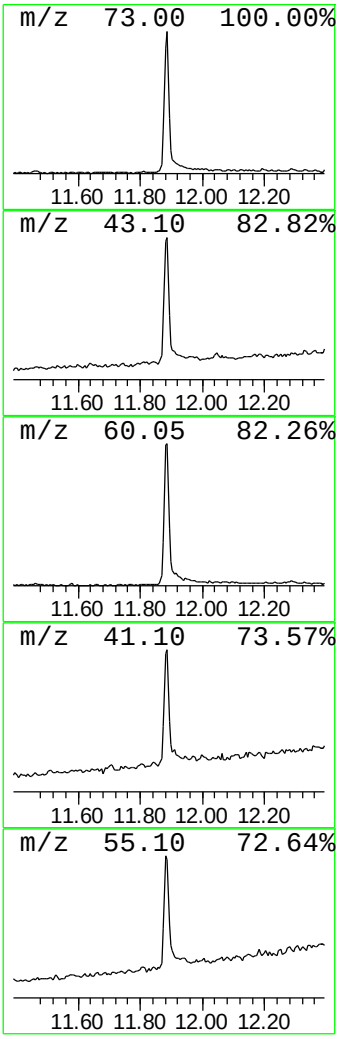
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	10.63 ng	641750	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020819\
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Acq On : 8 Feb 2019 15:30
Operator : JU/SJ
Sample : K1409-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

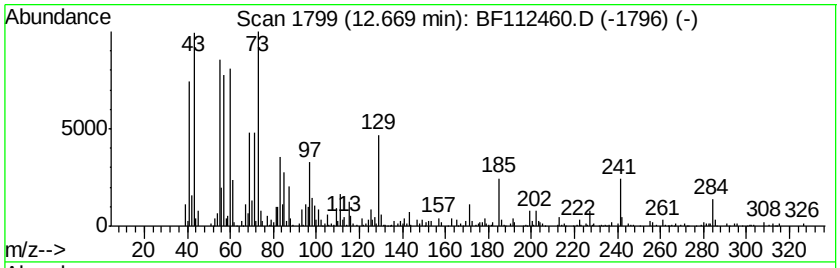
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

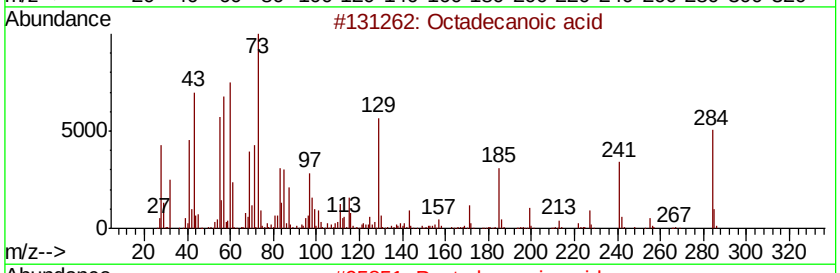
****

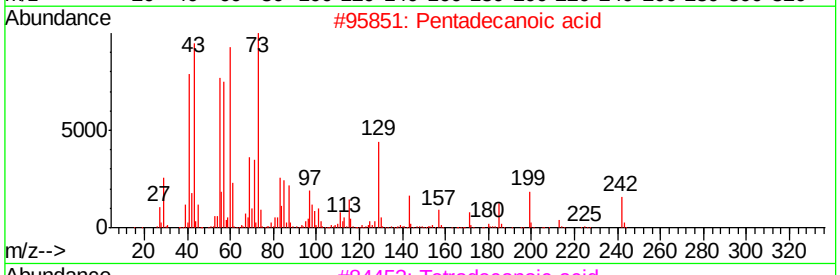
Peak Number 6 Octadecanoic acid Concentration Rank 5

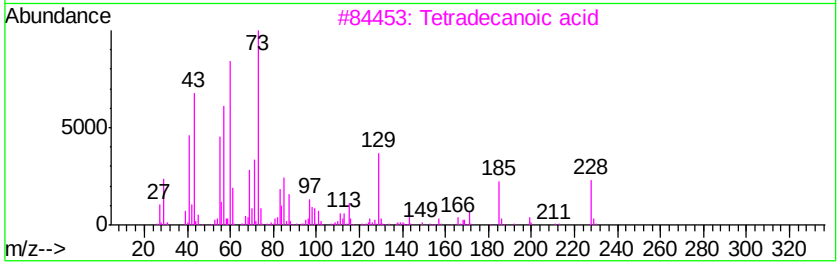
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	6.96 ng	420595	Phenanthrene-d10	11.36

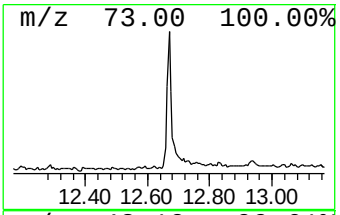
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Eicosanoic acid	312	C20H40O2	000506-30-9	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

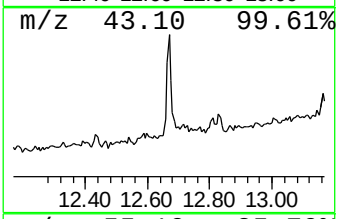


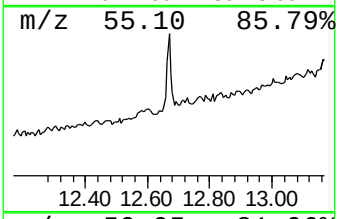


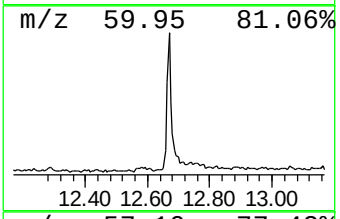


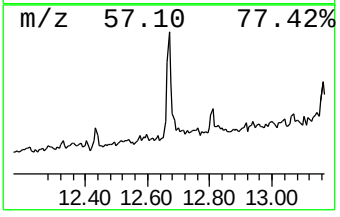












Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

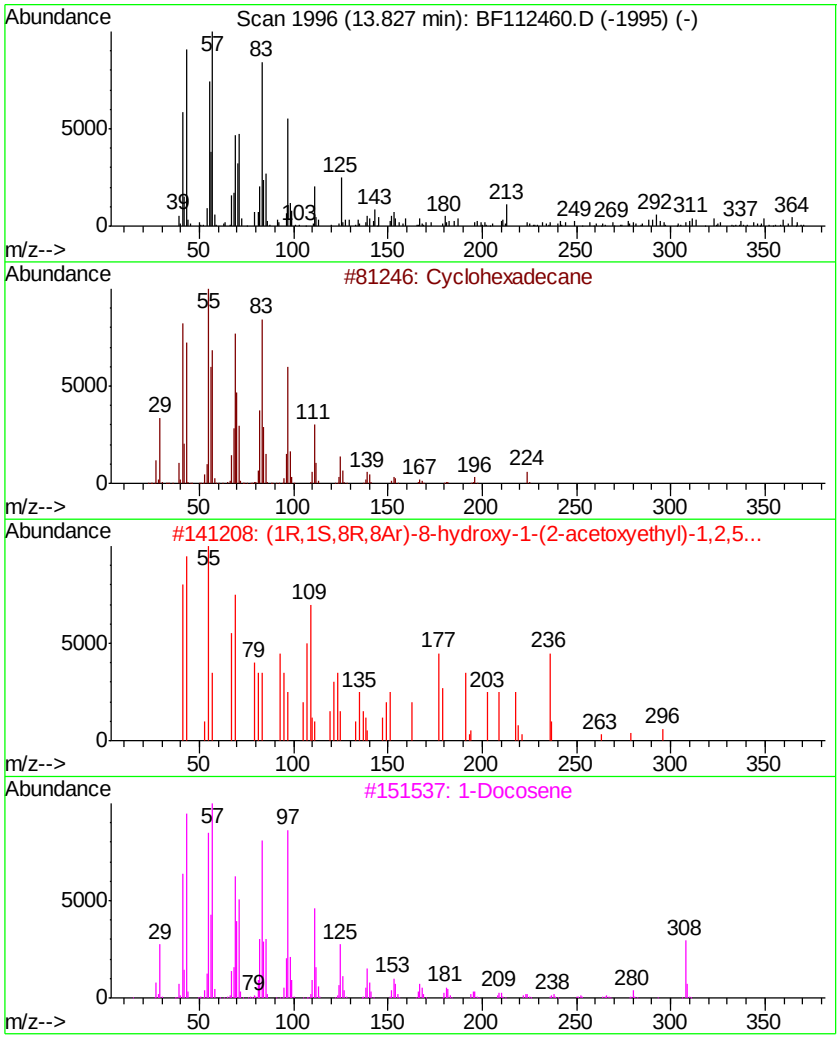
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

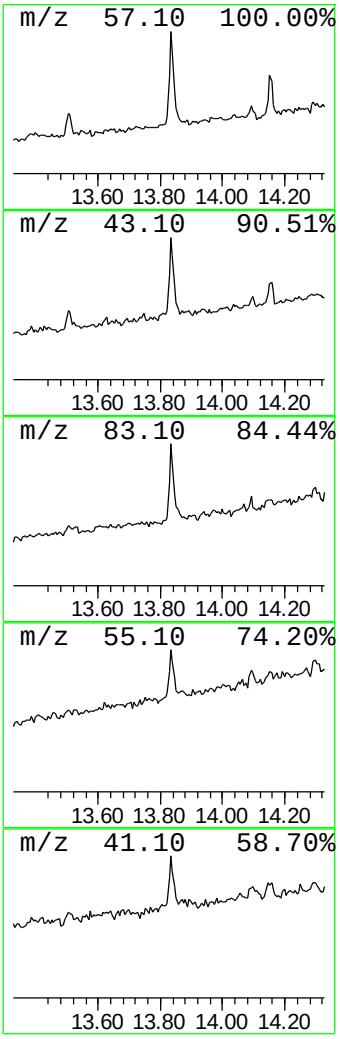
****

Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	8.42 ng	302479	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	(1R,1S,8R,8Ar)-8-hydroxy-1-(2-ac...	296	C18H32O3	1000298-98-5	90
3	1-Docosene	308	C22H44	001599-67-3	87
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	5.5	ng	230022	1	6.83	837944	20.0
2-Pentanone, 4-hy...	5.06	4.4	ng	183247	1	6.83	837944	20.0
unknown6.61	6.61	94.3	ng	3951780	1	6.83	837944	20.0
n-Hexadecanoic acid	11.89	10.6	ng	641750	4	11.36	1207900	20.0
Octadecanoic acid	12.67	7.0	ng	420595	4	11.36	1207900	20.0
Cyclohexadecane	13.83	8.4	ng	302479	5	14.01	718628	20.0