LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

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-BF012218.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	4.922	478	482	490	rVB	61441	85822	3.11%	0.368%
2	5.334	547	552	555	rBV	2668386	2612242	94.80%	11.215%
3	6.363	722	727	744	rBV	2625134	2755495	100.00%	11.830%
4	6.487	744	748	752	rBV	2781895	2712464	98.44%	11.646%
5	6.716	784	787	794	rBV	865530	725859	26.34%	3.116%
6	6.875	810	814	817	rBV	2453948	2146848	77.91%	9.217%
7	7.287	879	884	895	rBV	1665749	1657354	60.15%	7.116%
8	7.998	1001	1005	1021	rBV	986175	933450	33.88%	4.008%
9	9.075	1183	1188	1199	rBV	2961836	2707651	98.26%	11.625%
10	9.469	1250	1255	1264	rBV	220953	214314	7.78%	0.920%
11	9.680	1288	1291	1295	rBV	40210	32877	1.19%	0.141%
12	9.751	1299	1303	1312	rVV	903162	795382	28.87%	3.415%
13	10.180	1373	1376	1379	rVB	37597	28717	1.04%	0.123%
14	10.463	1420	1424	1430	rBV	32037	37095	1.35%	0.159%
15	10.545	1434	1438	1453	rVB	1108357	1148474	41.68%	4.931%
16	11.239	1552	1556	1559	rBV	693487	638672	23.18%	2.742%
17	12.821	1821	1825	1829	rBV	2147501	2077428	75.39%	8.919%
18	13.033	1858	1861	1866	rBV6	17120	29831	1.08%	0.128%
19	13.716	1974	1977	1985	rBV	255985	343232	12.46%	1.474%
20	13.880	2001	2005	2012	rVB	714661	742568	26.95%	3.188%
21	13.968	2017	2020	2024	rVV	75002	71194	2.58%	0.306%
22	14.357	2084	2086	2091	rVB5	38251	40289	1.46%	0.173%
23	14.780	2155	2158	2161	rVB2	68501	65771	2.39%	0.282%
24	14.957	2186	2188	2191	rVB	34365	33798	1.23%	0.145%
25	15.310	2243	2248	2257	rVB	410133	567675	20.60%	2.437%
26	15.509	2279	2282	2287	rVB2	74348	87360	3.17%	0.375%

Sum of corrected areas: 23291862

LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
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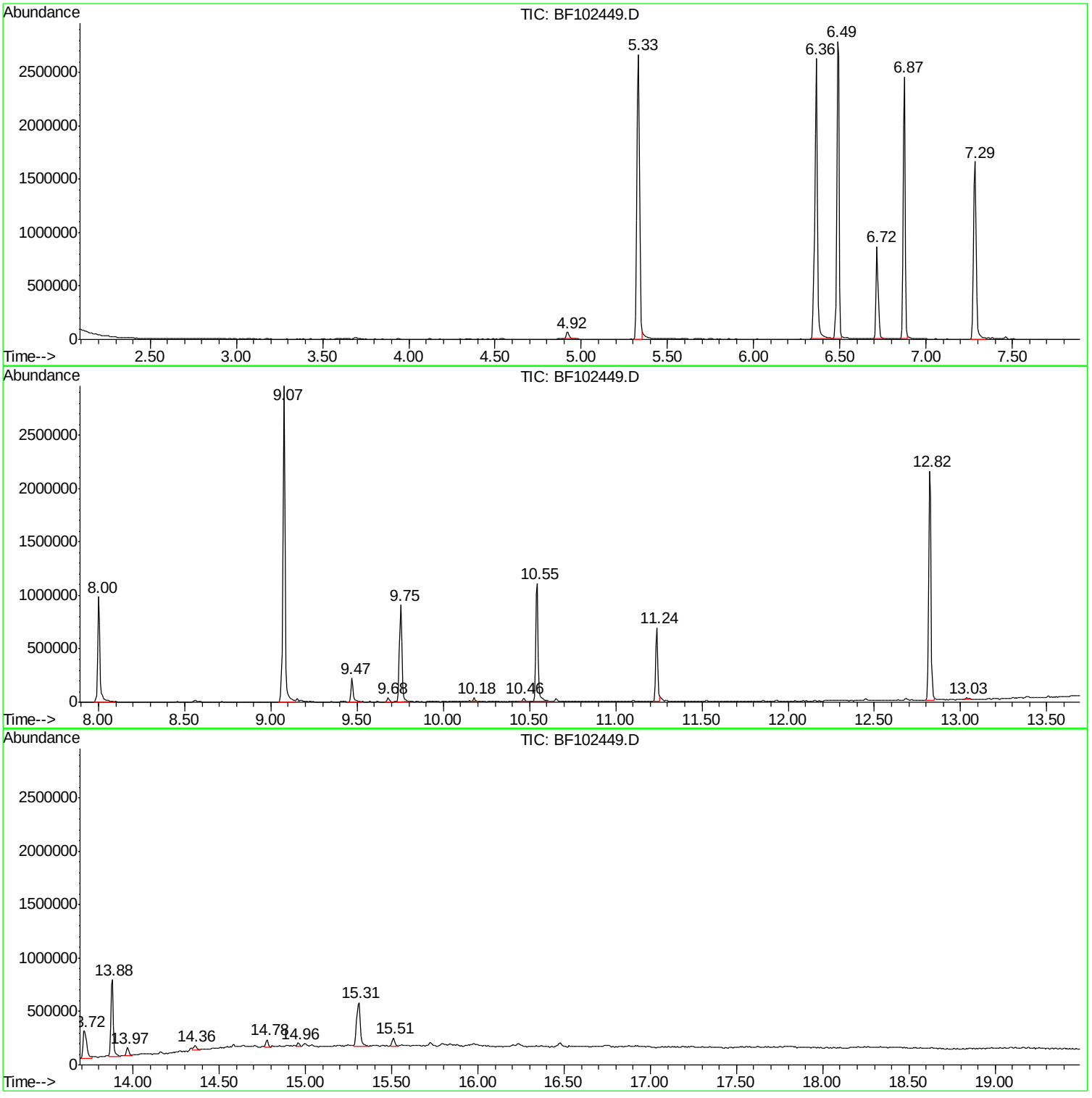
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

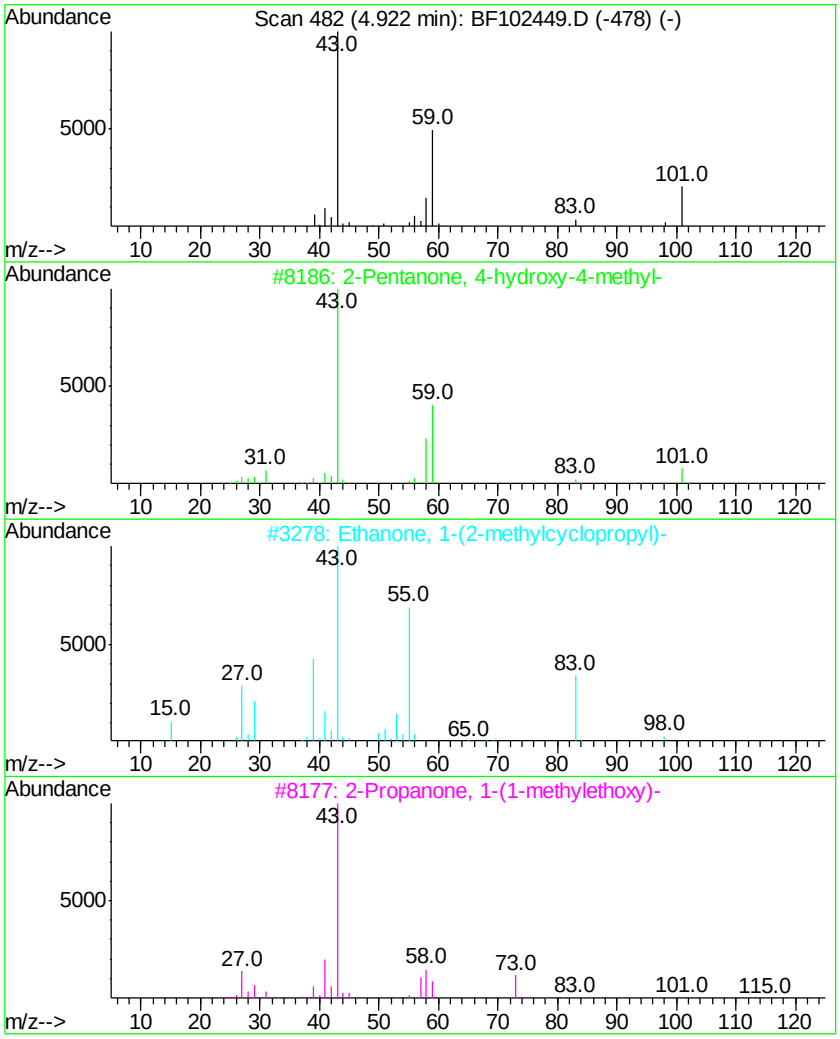
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

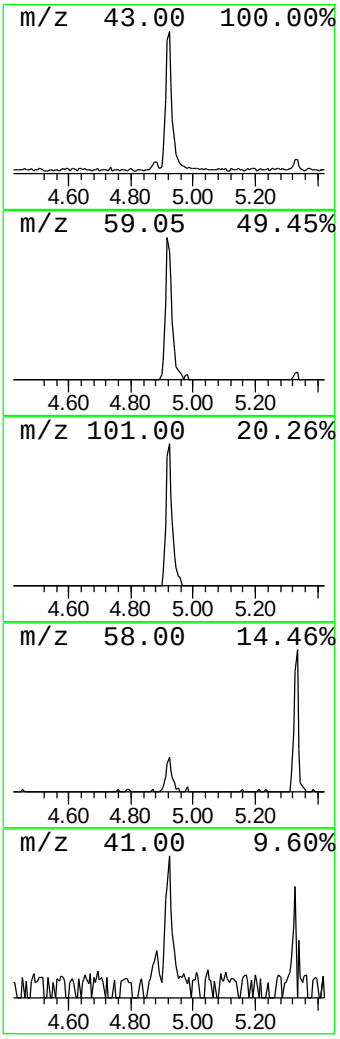
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.36 ng	85822	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
3	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

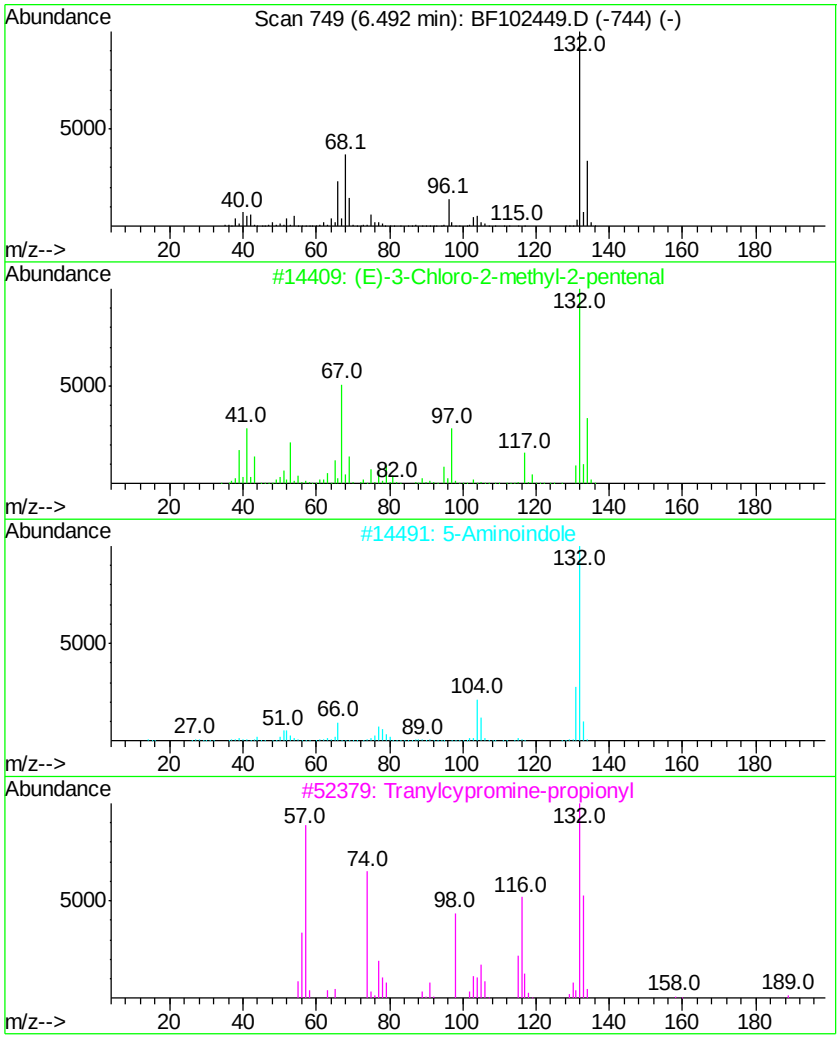
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

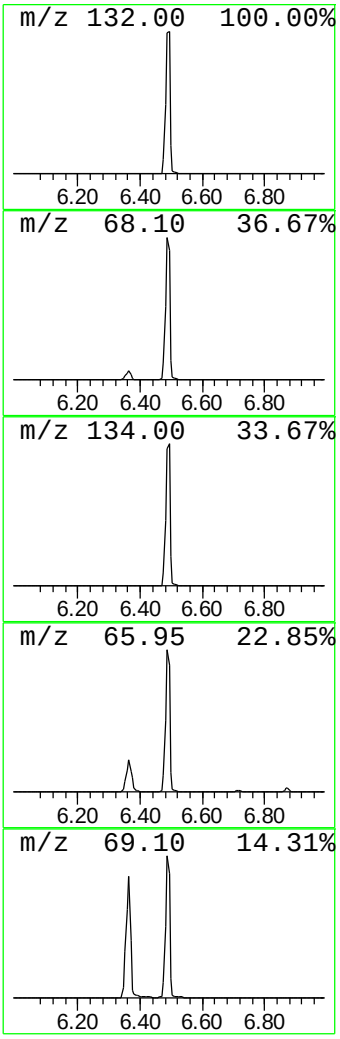
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	74.74 ng	2712460	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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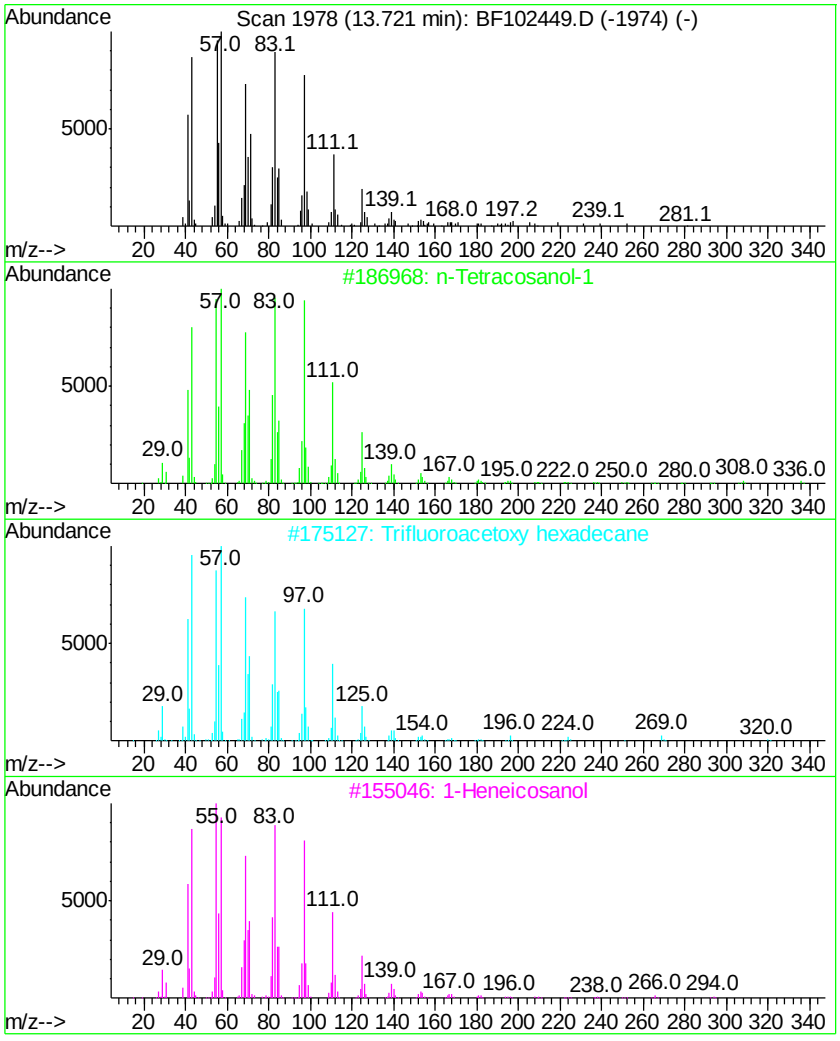
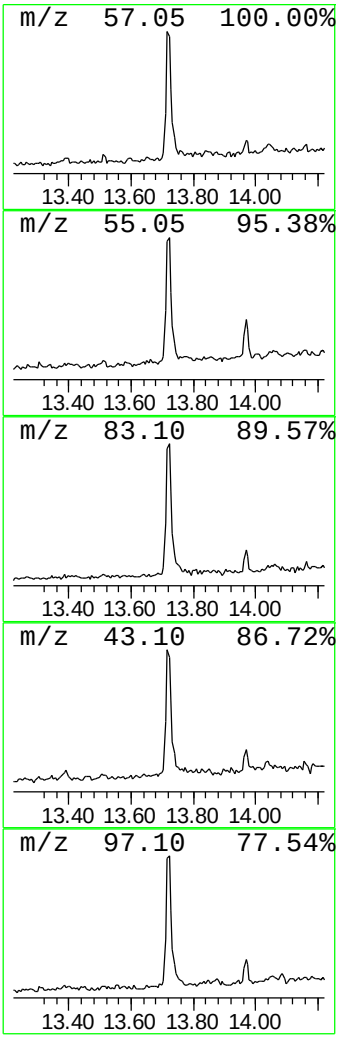
Peak Number 4 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.24 ng	343232	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

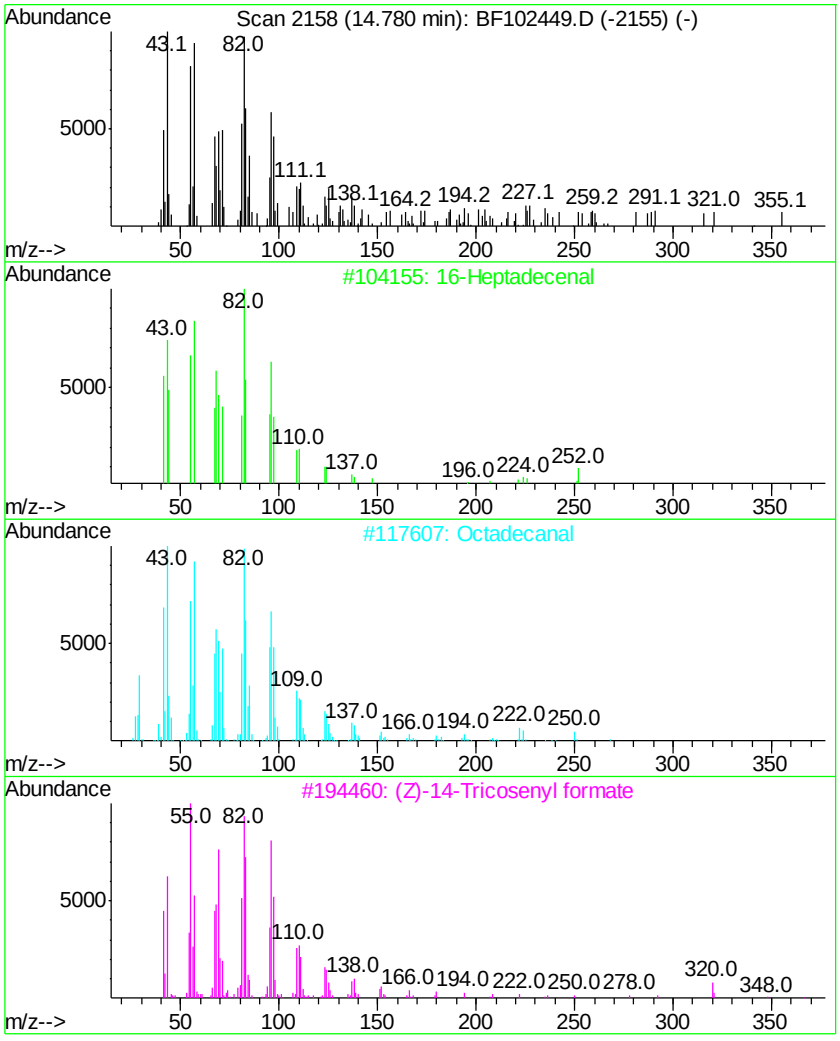
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

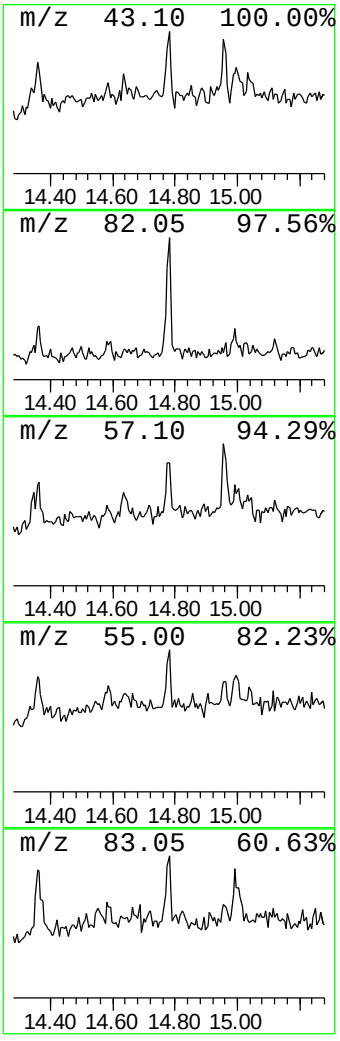
****

Peak Number 5 16-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.32 ng	65771	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1000144-57-9	86
2	Octadecanal	268	C18H36O	000638-66-4	80
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	70
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	52





Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
Operator : SJ/JU
Sample : J1289-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

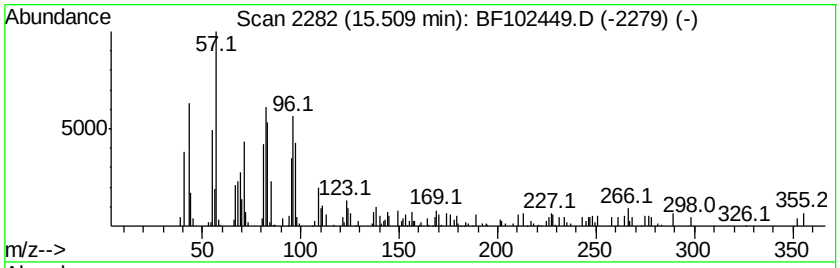
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

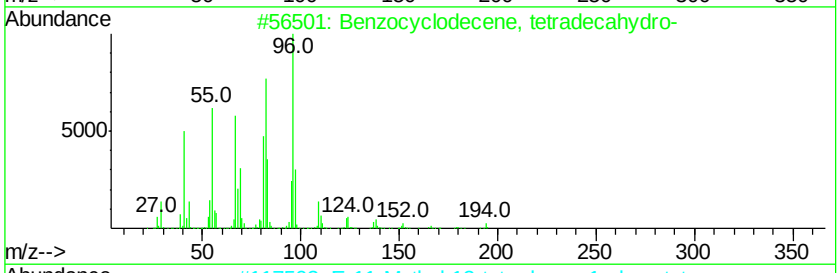
****

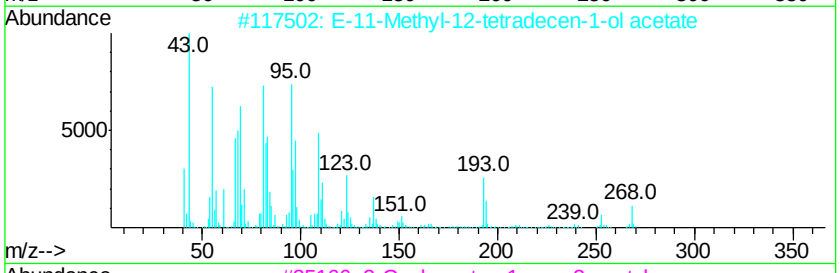
Peak Number 6 unknown15.51 Concentration Rank 4

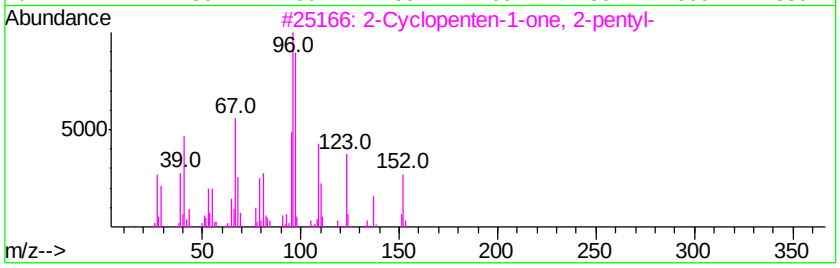
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	3.08 ng	87360	Perylene-d12	15.31

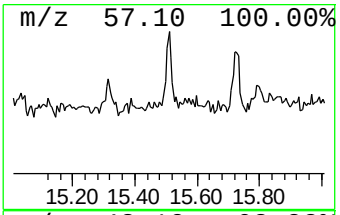
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocyclodecene, tetradecahydro-	194	C14H26	061142-06-1	42
2	E-11-Methyl-12-tetradecen-1-ol a...	268	C17H32O2	1000130-80-7	35
3	2-Cyclopenten-1-one, 2-pentyl-	152	C10H16O	025564-22-1	30
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	27
5	Spiro[4.5]decane	138	C10H18	000176-63-6	27

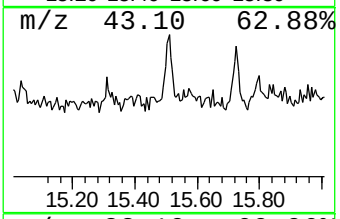


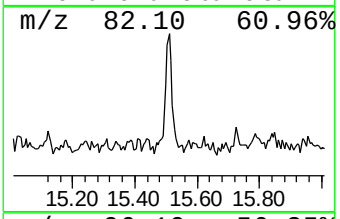


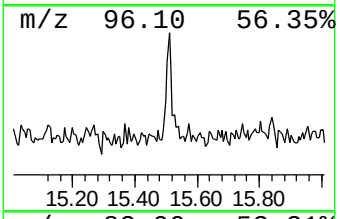


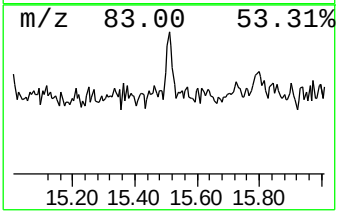












Tentatively Identified Compound (LSC) summary

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Data File : BF102449.D
Acq On : 26 Jan 2018 2:52
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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...	4.92	2.4	ng	85822	1	6.72	725859	20.0
unknown6.49	6.49	74.7	ng	2712460	1	6.72	725859	20.0
n-Tetracosanol-1	13.72	9.2	ng	343232	5	13.88	742568	20.0
16-Heptadecenal	14.78	2.3	ng	65771	6	15.31	567675	20.0
unknown15.51	15.51	3.1	ng	87360	6	15.31	567675	20.0