LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-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-BF121918.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	2.240	23	26	31	rVB	65990	92421	1.84%	0.215%
2	5.128	511	517	523	rBV	194946	251468	5.01%	0.585%
3	5.522	579	584	587	rBV	4332578	4472546	89.03%	10.409%
4	6.522	748	754	759	rBV	4400813	4965882	98.85%	11.557%
5	6.669	774	779	782	rBV	4972815	4625482	92.07%	10.764%
6	6.898	814	818	821	rBV	1489574	1277875	25.44%	2.974%
7	7.057	840	845	848	rBV	3902697	3701703	73.68%	8.615%
8	7.451	907	912	915	rBV	2993434	2935041	58.42%	6.830%
9	8.175	1031	1035	1039	rBV	1885473	1593239	31.71%	3.708%
10	8.792	1135	1140	1144	rBV	1956036	1637972	32.60%	3.812%
11	9.251	1213	1218	1221	rBV	5727848	5023818	100.00%	11.691%
12	9.639	1280	1284	1287	rBV	294381	220720	4.39%	0.514%
13	9.928	1329	1333	1337	rVB	1705605	1602956	31.91%	3.730%
14	10.716	1462	1467	1470	rBV	2831512	2460197	48.97%	5.725%
15	11.410	1582	1585	1589	rBV	1463470	1317121	26.22%	3.065%
16	11.933	1671	1674	1686	rVB	138785	144188	2.87%	0.336%
17	12.998	1850	1855	1858	rBV	3972031	3612451	71.91%	8.407%
18	13.886	2003	2006	2012	rBV	154459	178808	3.56%	0.416%
19	14.045	2029	2033	2036	rBV	1607453	1431194	28.49%	3.331%
20	14.521	2111	2114	2117	rBV	63187	60213	1.20%	0.140%
21	15.174	2222	2225	2232	rVB	69838	94870	1.89%	0.221%
22	15.521	2279	2284	2288	rVV	832510	1050063	20.90%	2.444%
23	15.568	2288	2292	2297	rVB	65148	99586	1.98%	0.232%
24	16.010	2363	2367	2372	rBV	77655	120305	2.39%	0.280%

Sum of corrected areas: 42970119

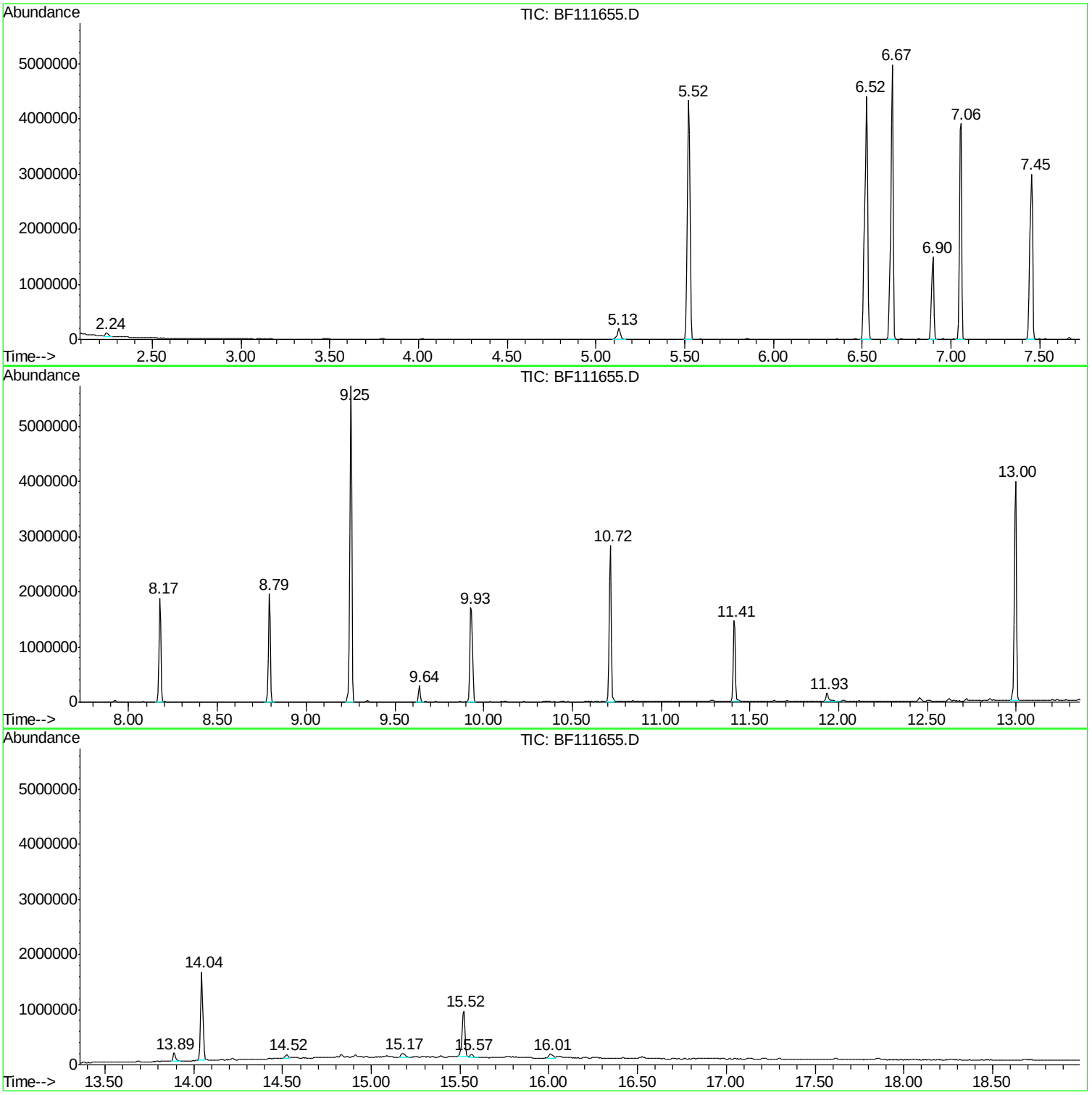
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

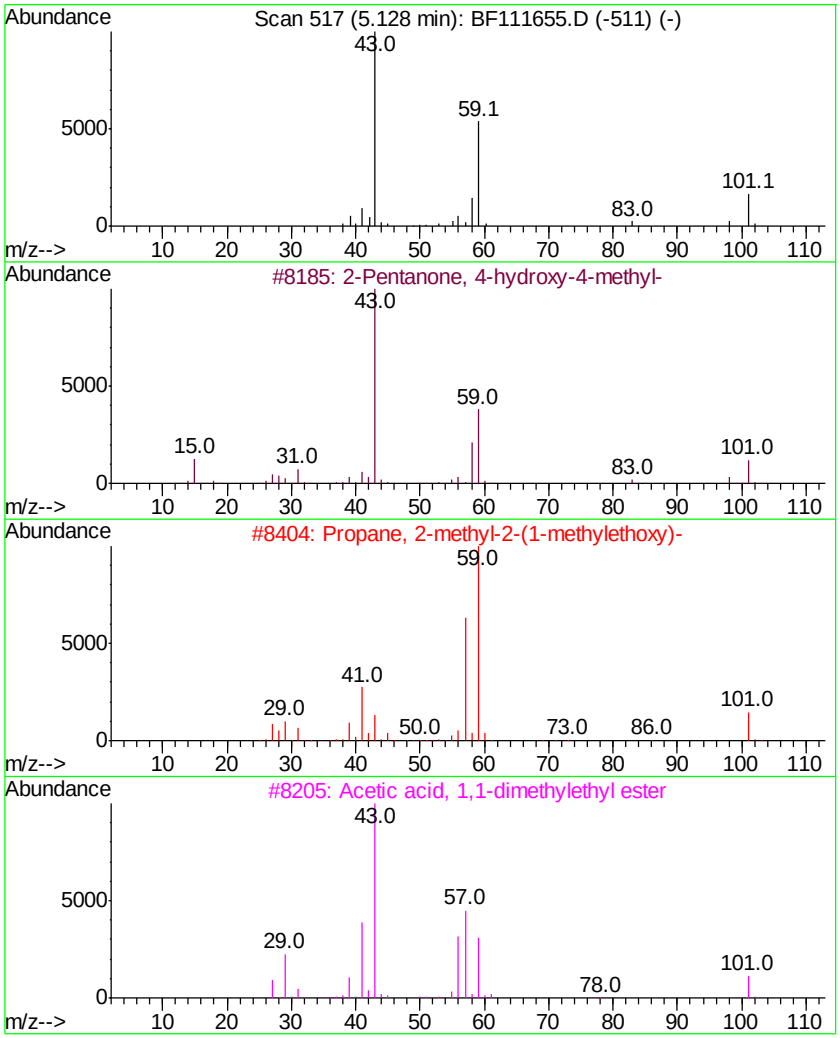
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

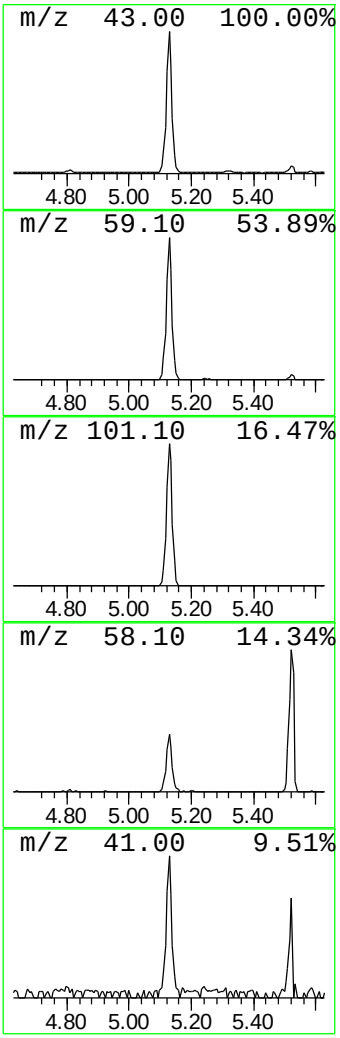
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.94 ng	251468	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

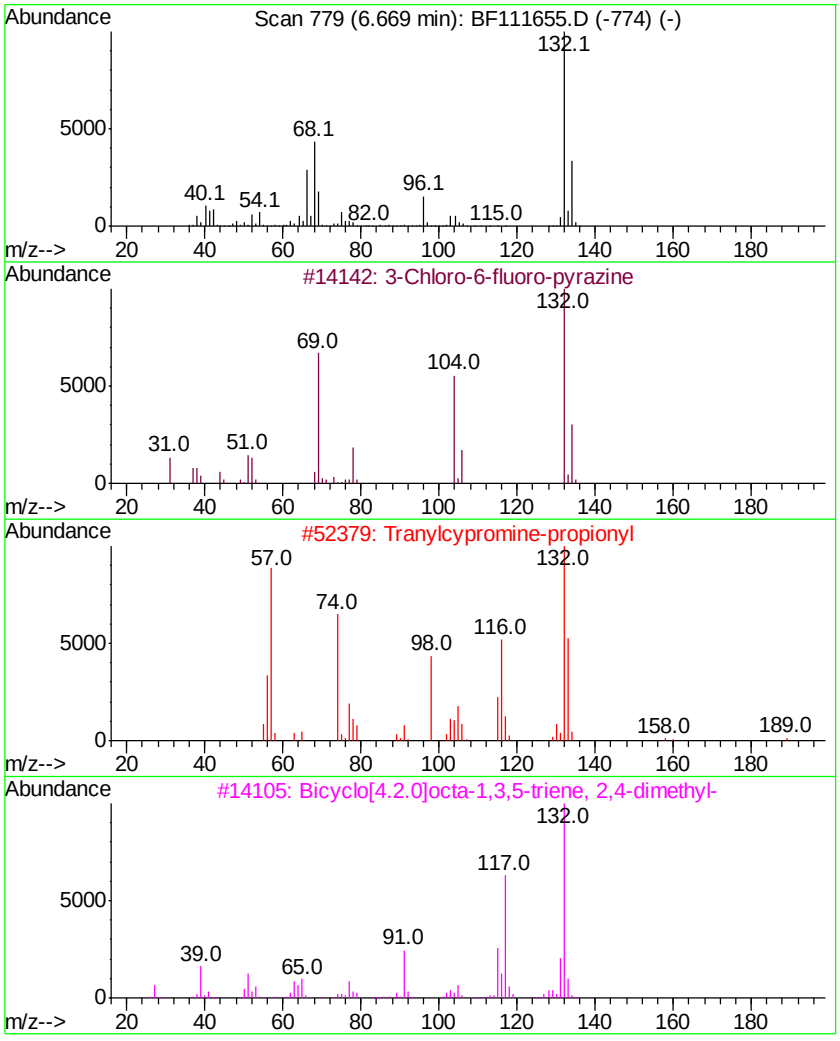
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

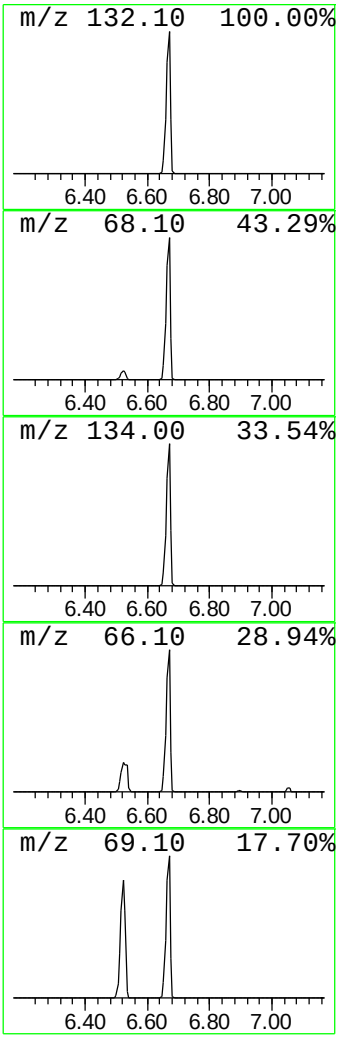
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	72.39 ng	4625480	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

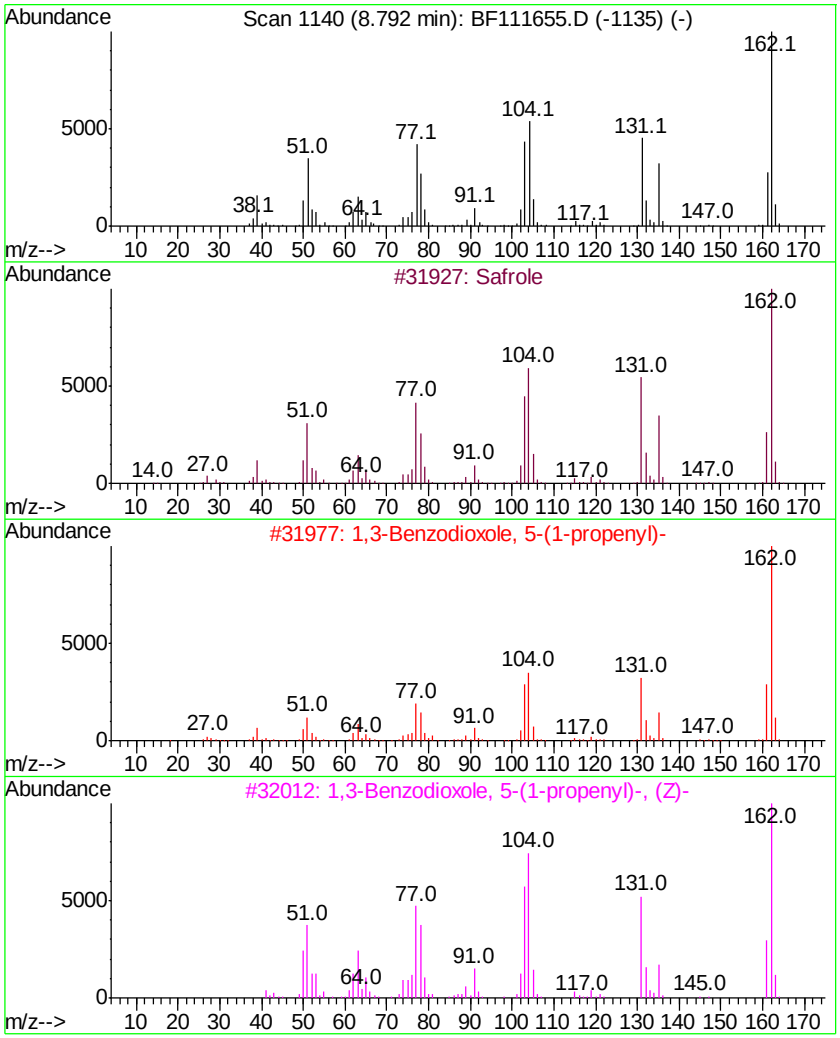
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

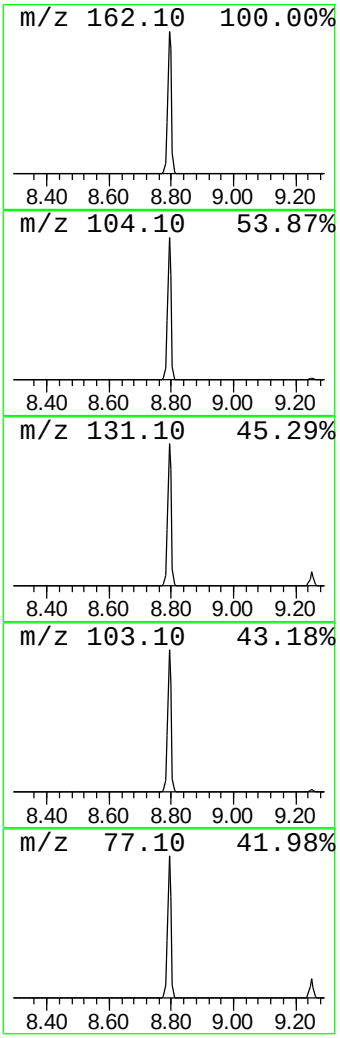
****

Peak Number 4 Safrole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	20.56 ng	1637970	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	94
4	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	94
5	1H-Isoindole-1,3(2H)-dione, 2-am...	162	C8H6N2O2	001875-48-5	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

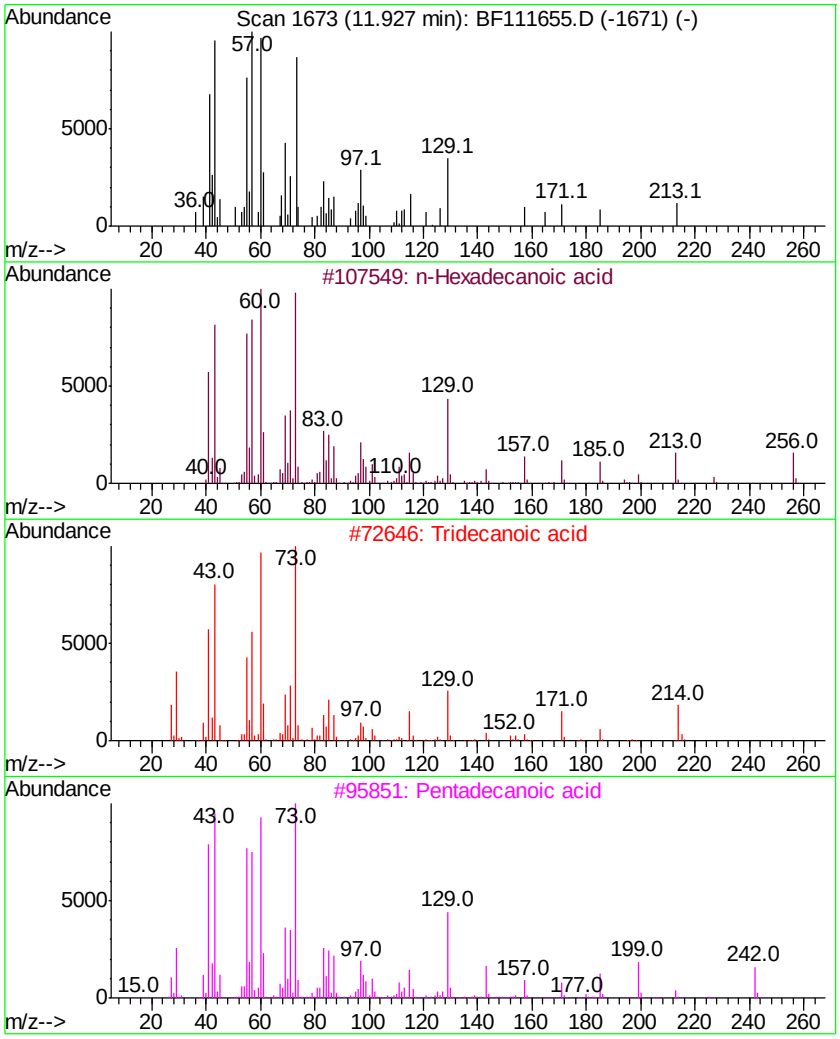
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

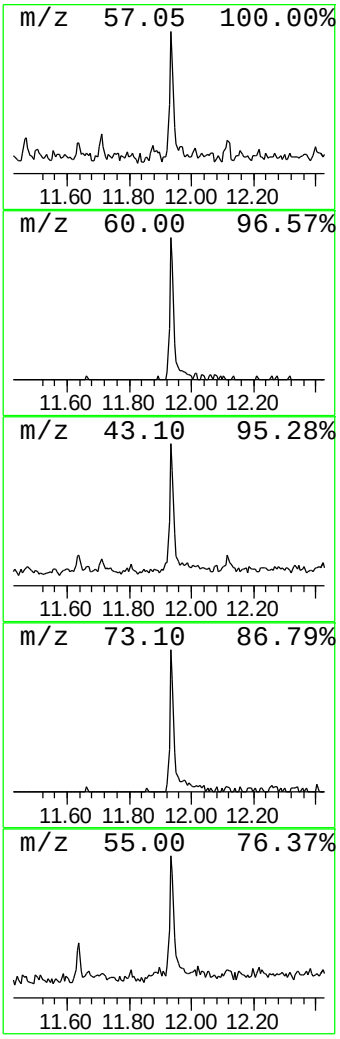
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.19 ng	144188	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

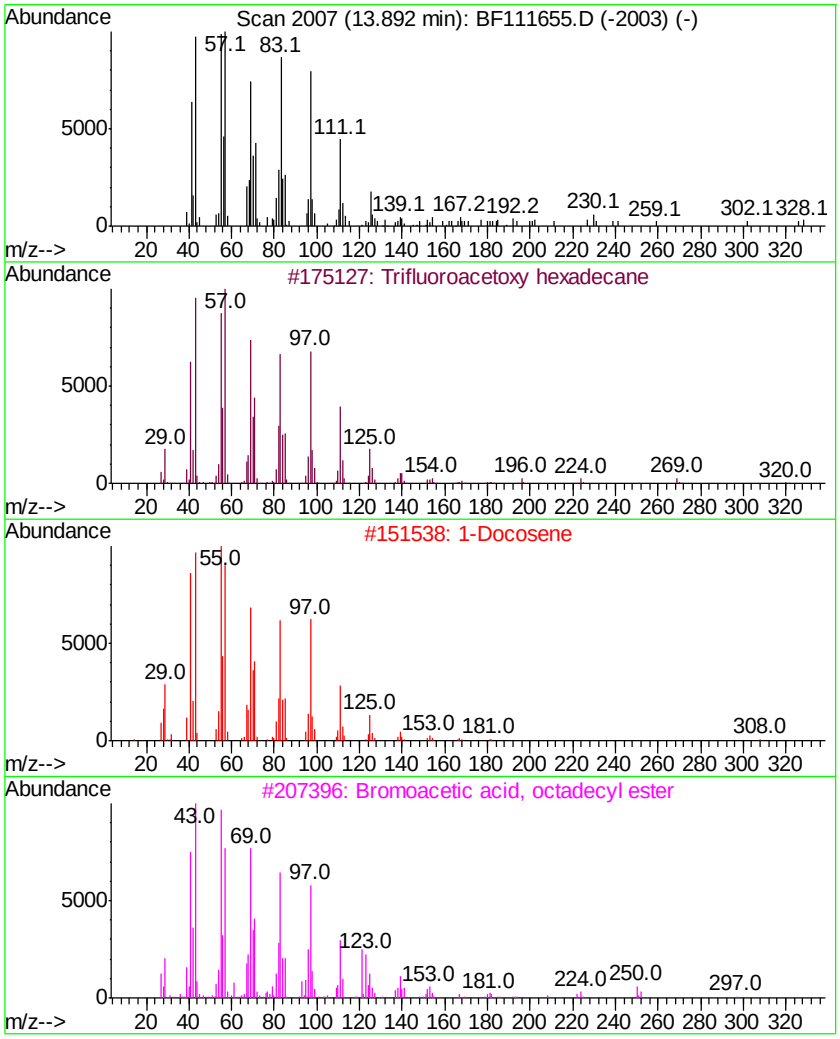
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

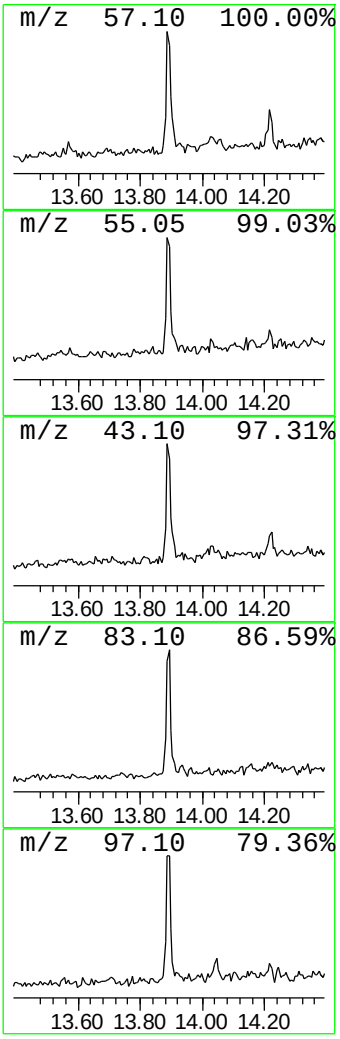
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.50 ng	178808	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	1-Docosene	308	C22H44	001599-67-3	93
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	93
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
5	Octacosanol	410	C28H58O	000557-61-9	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

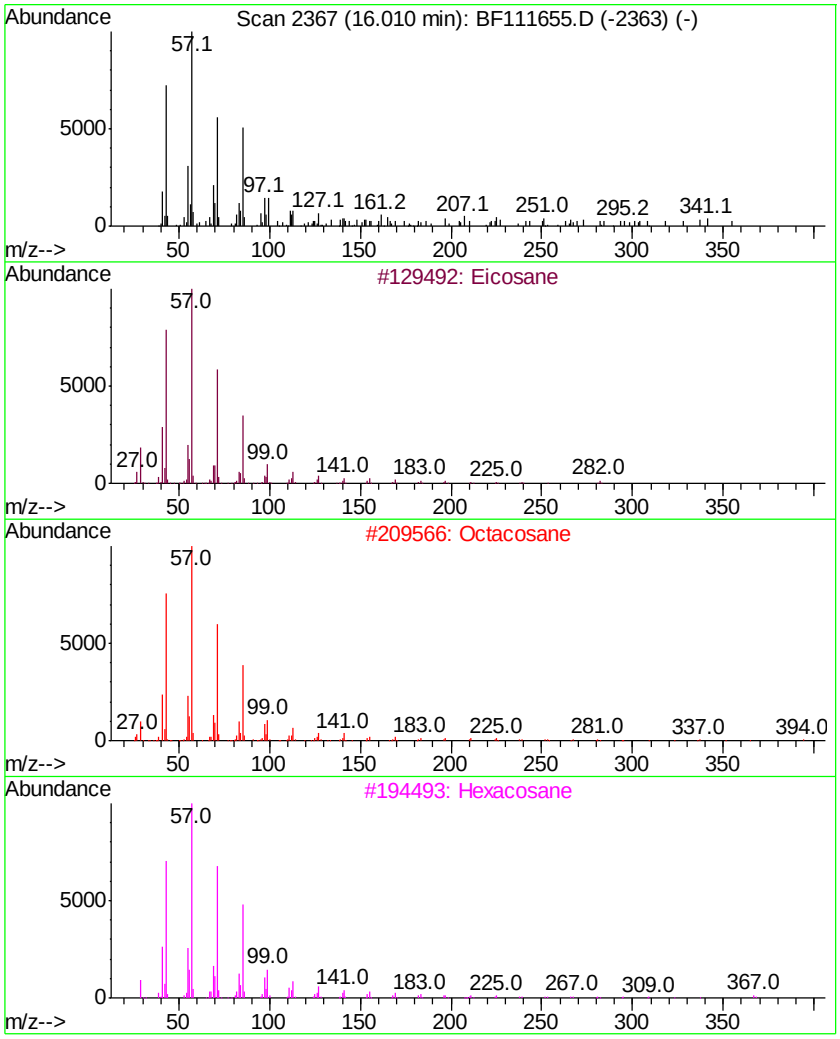
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

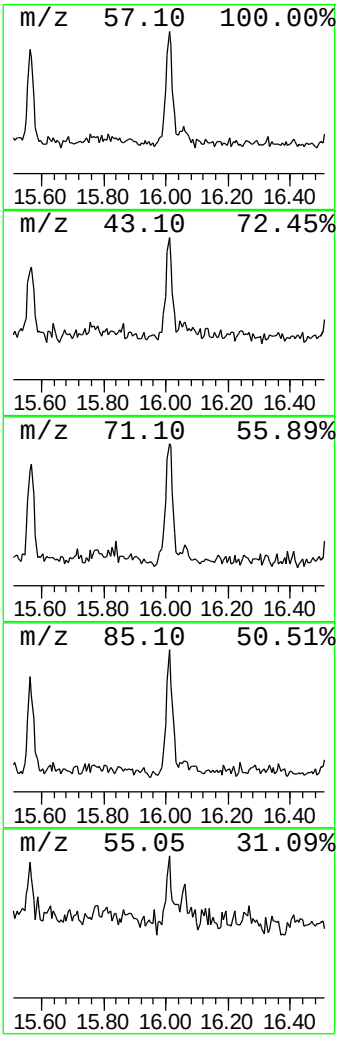
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	2.29 ng	120305	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	92
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122018\
Data File : BF111655.D
Acq On : 20 Dec 2018 22:50
Operator : JU/SJ
Sample : J6362-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	5.13	3.9	ng	251468	1	6.90	1277880	20.0
unknown6.67	6.67	72.4	ng	4625480	1	6.90	1277880	20.0
Safrole	8.79	20.6	ng	1637970	2	8.17	1593240	20.0
n-Hexadecanoic acid	11.93	2.2	ng	144188	4	11.41	1317120	20.0
Trifluoroacetoxy ...	13.89	2.5	ng	178808	5	14.04	1431190	20.0
Eicosane	16.01	2.3	ng	120305	6	15.52	1050060	20.0