LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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	4.898	475	478	491	rBV	39654	61513	3.15%	0.357%
2	5.322	546	550	587	rBV	1068186	1664361	85.10%	9.671%
3	6.345	721	724	741	rBV	1186771	1858768	95.04%	10.801%
4	6.469	741	745	770	rVB	1641628	1955851	100.00%	11.365%
5	6.698	780	784	795	rBV	428325	585721	29.95%	3.404%
6	6.816	801	804	807	rVB	57435	42550	2.18%	0.247%
7	6.851	807	810	843	rVB	1309931	1463197	74.81%	8.503%
8	7.257	876	879	910	rBV	765479	1182477	60.46%	6.871%
9	7.975	998	1001	1027	rBV	574683	763193	39.02%	4.435%
10	9.051	1180	1184	1210	rBV	1814465	1920862	98.21%	11.162%
11	9.445	1247	1251	1266	rBV	104735	123661	6.32%	0.719%
12	9.722	1294	1298	1320	rBV	726562	717850	36.70%	4.171%
13	10.510	1428	1432	1450	rBV	718423	906933	46.37%	5.270%
14	11.198	1546	1549	1570	rBV	453826	592723	30.31%	3.444%
15	12.610	1785	1789	1792	rBV3	18439	21234	1.09%	0.123%
16	12.674	1795	1800	1814	rVB	35963	79479	4.06%	0.462%
17	12.780	1814	1818	1829	rBV	1361968	1350056	69.03%	7.845%
18	13.263	1892	1900	1906	rBV	286442	314217	16.07%	1.826%
19	13.686	1969	1972	1989	rBV3	51045	110459	5.65%	0.642%
20	13.827	1992	1996	2005	rBV	573729	603691	30.87%	3.508%
21	13.998	2021	2025	2028	rBV	31761	28371	1.45%	0.165%
22	14.304	2073	2077	2079	rBV	35572	34916	1.79%	0.203%
23	14.592	2121	2126	2132	rVB	44440	47783	2.44%	0.278%
24	14.904	2175	2179	2182	rBV	56219	55228	2.82%	0.321%
25	15.221	2228	2233	2247	rVB	397218	587634	30.04%	3.415%
26	15.645	2301	2305	2310	rBV	43504	58798	3.01%	0.342%
27	16.104	2378	2383	2394	rVB4	25507	52790	2.70%	0.307%
28	16.633	2470	2473	2480	rVB3	13413	24651	1.26%	0.143%

Sum of corrected areas: 17208967

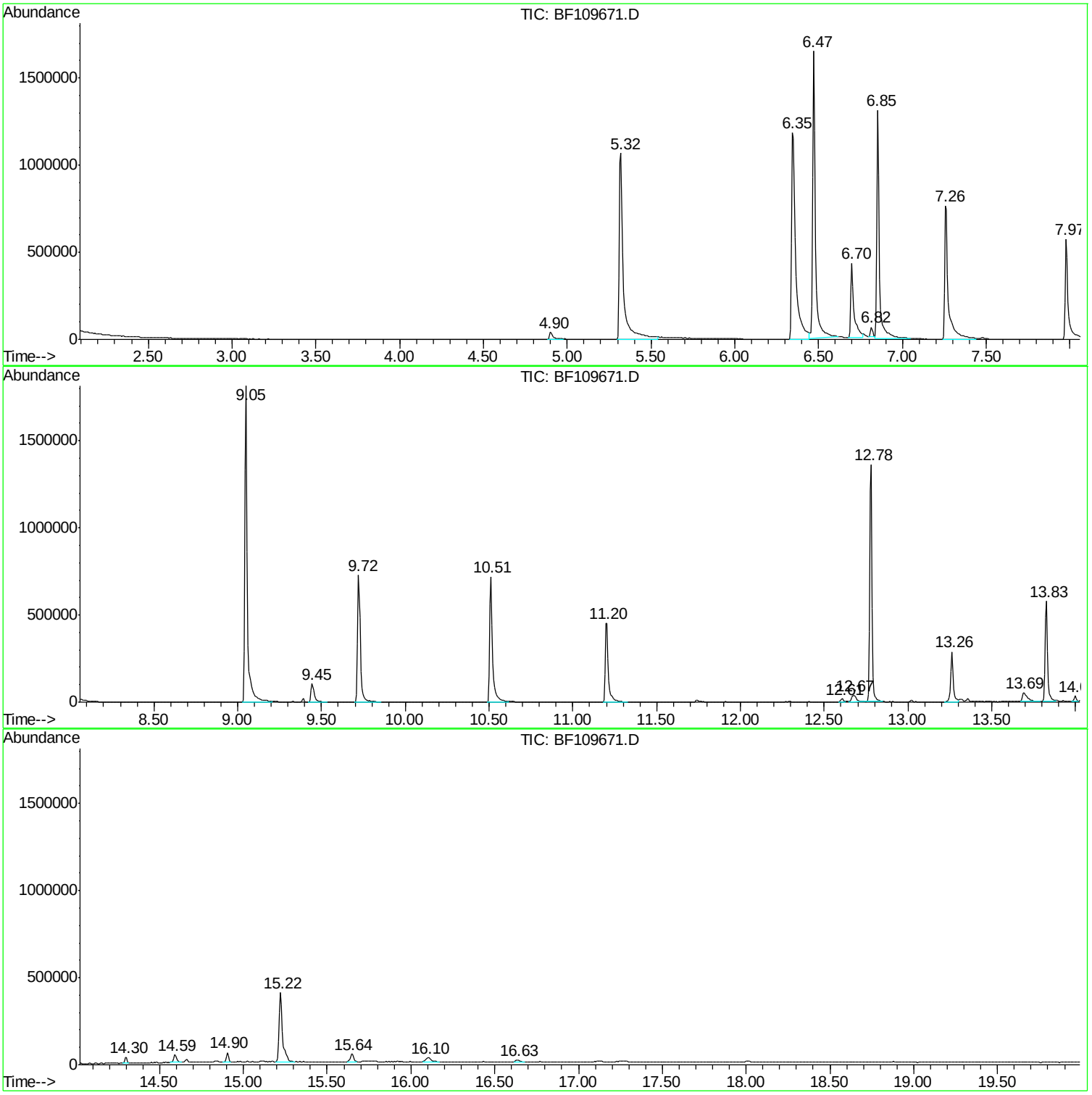
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-6

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\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

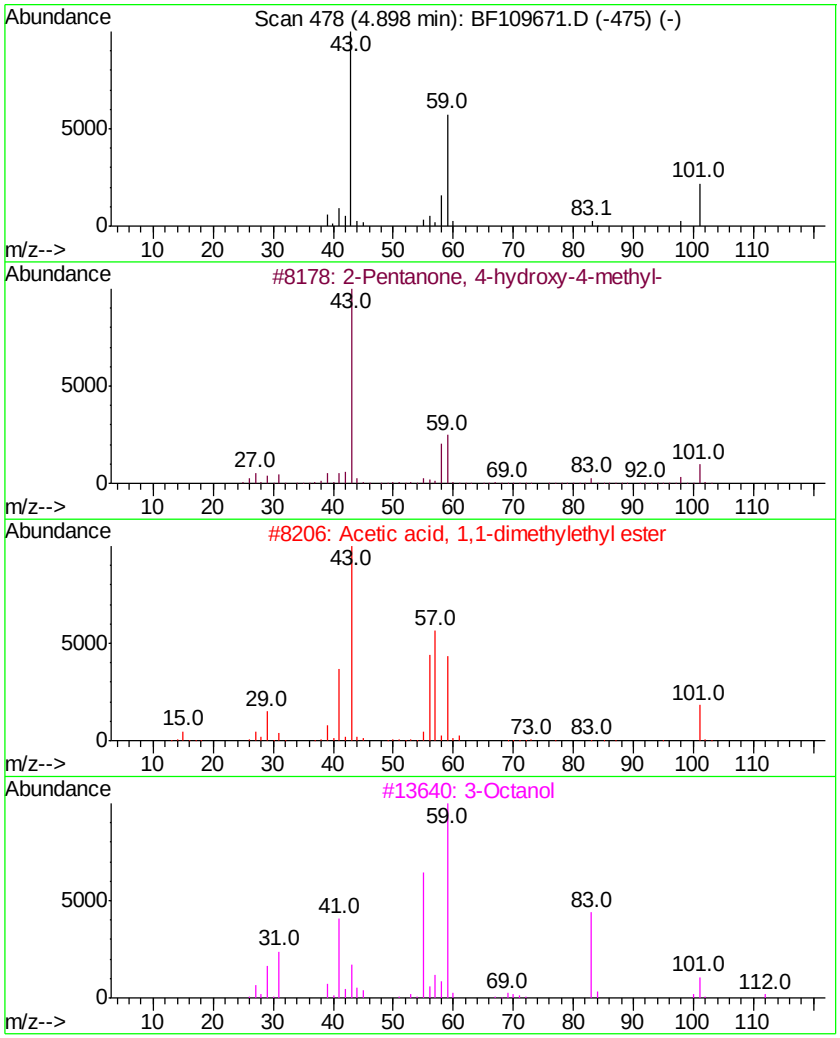
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

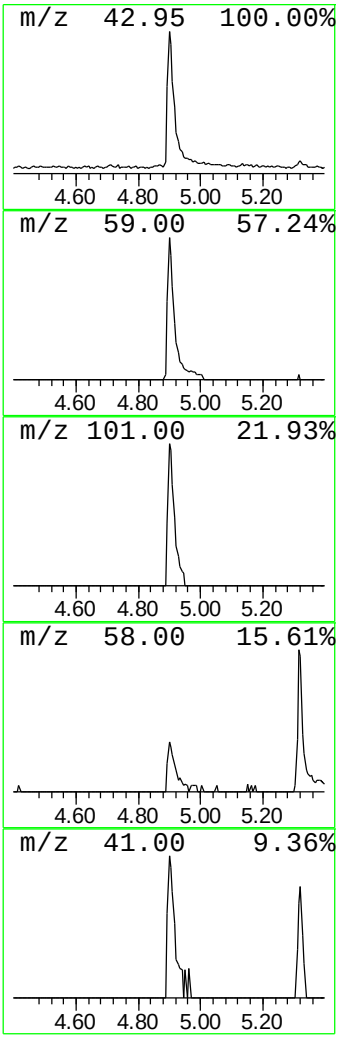
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.10 ng	61513	1,4-Dichlorobenzene-d4	6.70

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	3-Octanol	130	C8H18O	000589-98-0	25
4	Acetone	58	C3H6O	000067-64-1	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

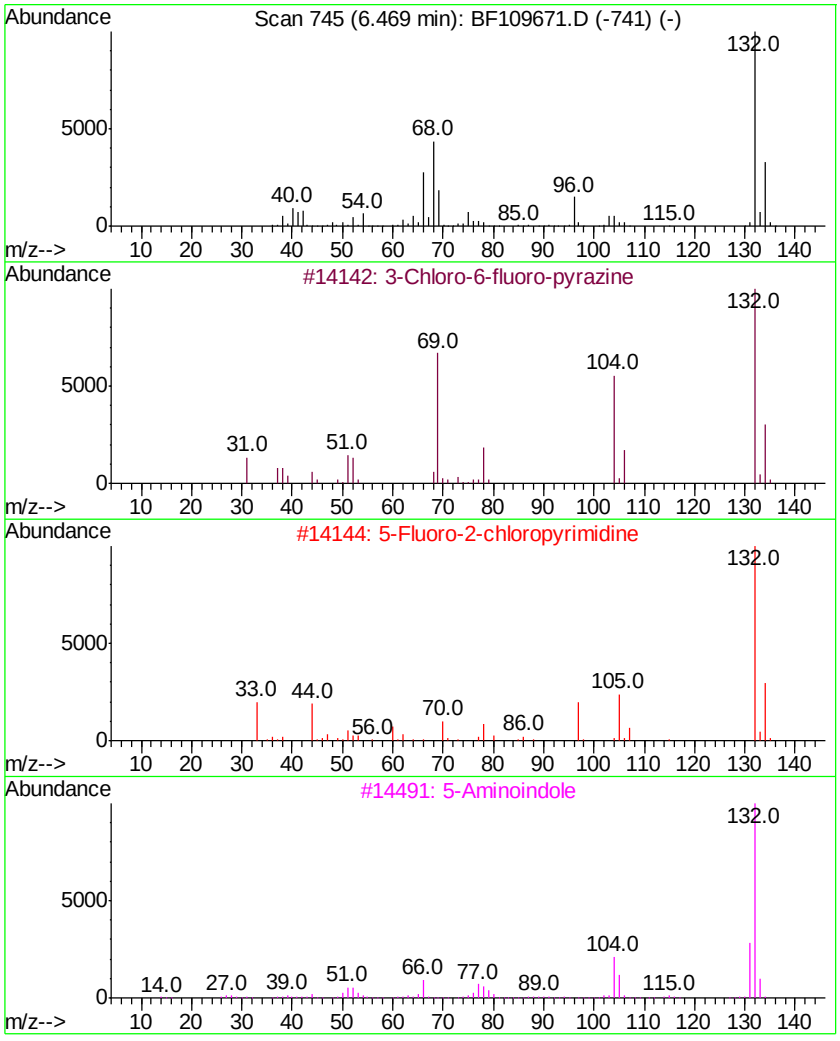
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

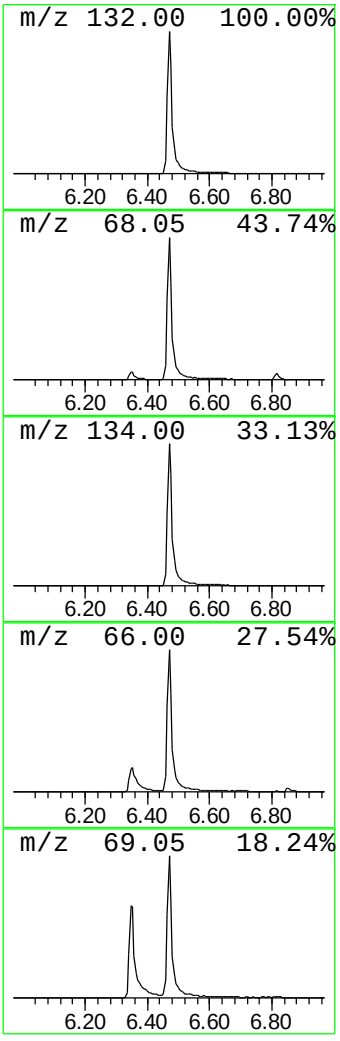
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	66.78 ng	1955850	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

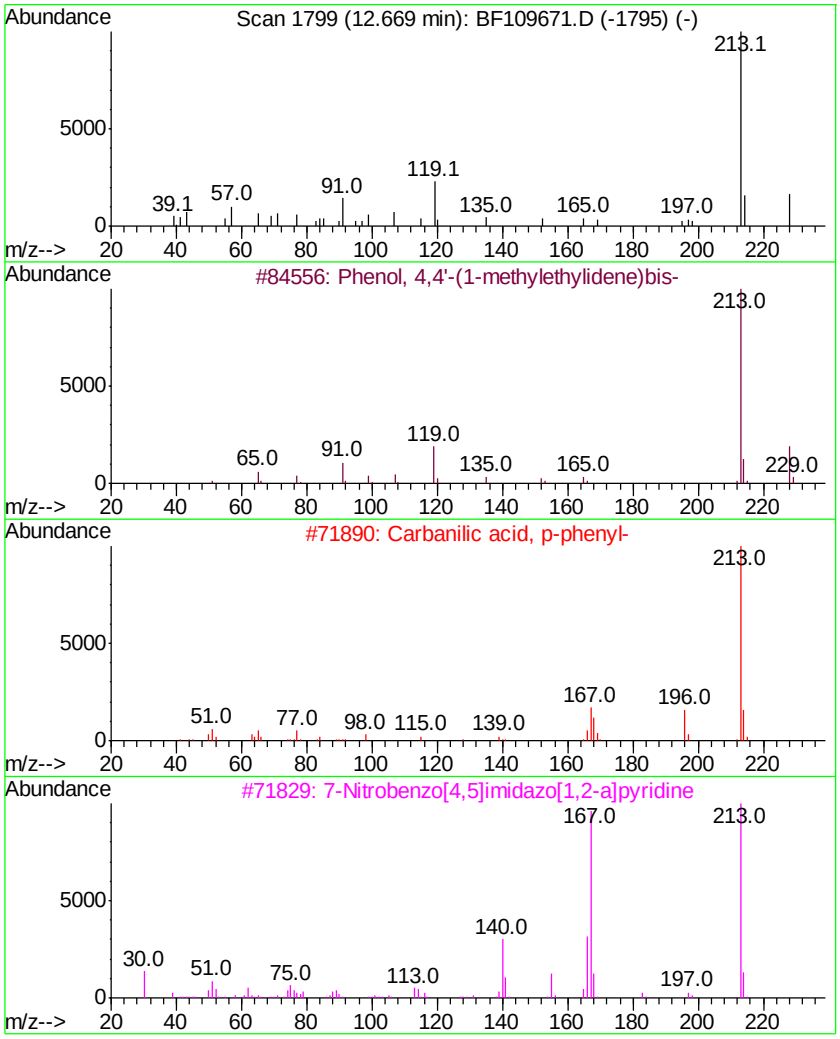
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

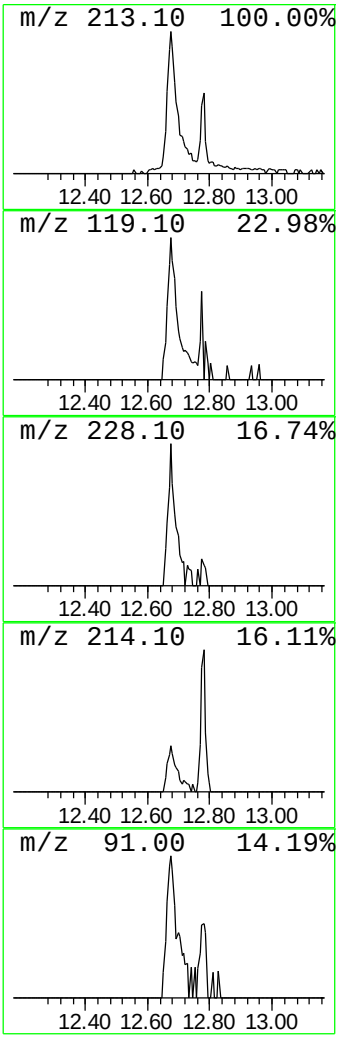
****

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.63 ng	79479	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	46
3	7-Nitrobenzo[4,5]imidazo[1,2-a]p...	213	C11H7N3O2	1000322-50-9	38
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	37
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	33





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

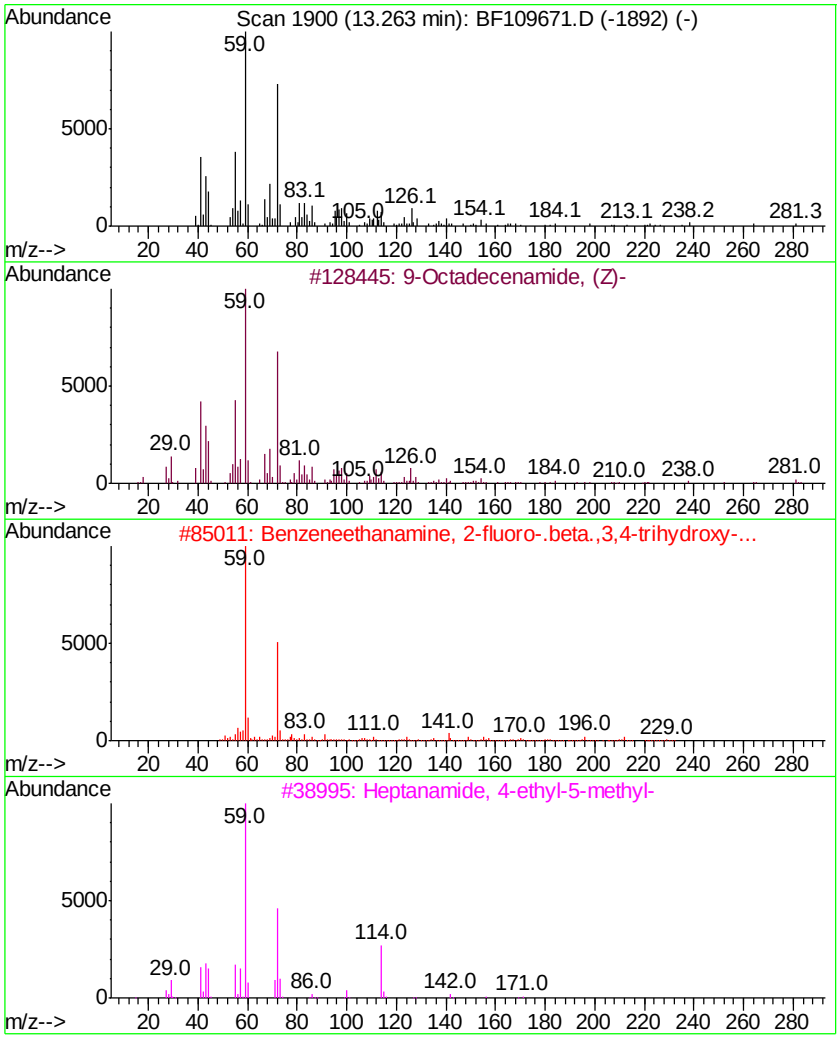
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

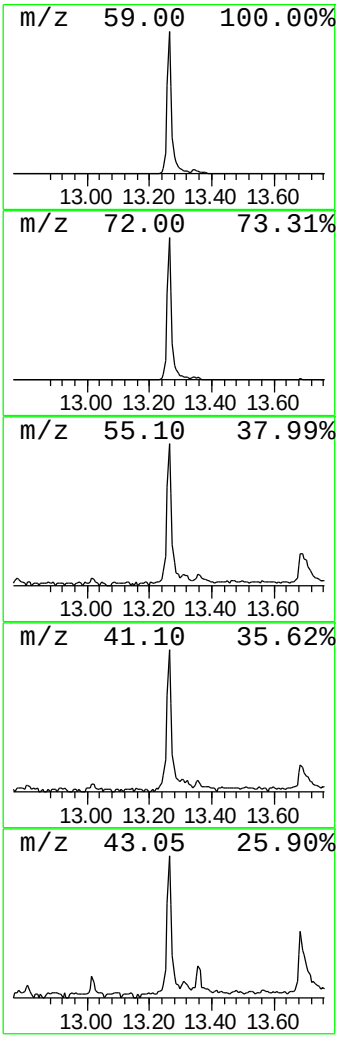
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	10.41 ng	314217	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
4	Hexadecanamide	255	C16H33NO	000629-54-9	56
5	Octanamide	143	C8H17NO	000629-01-6	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

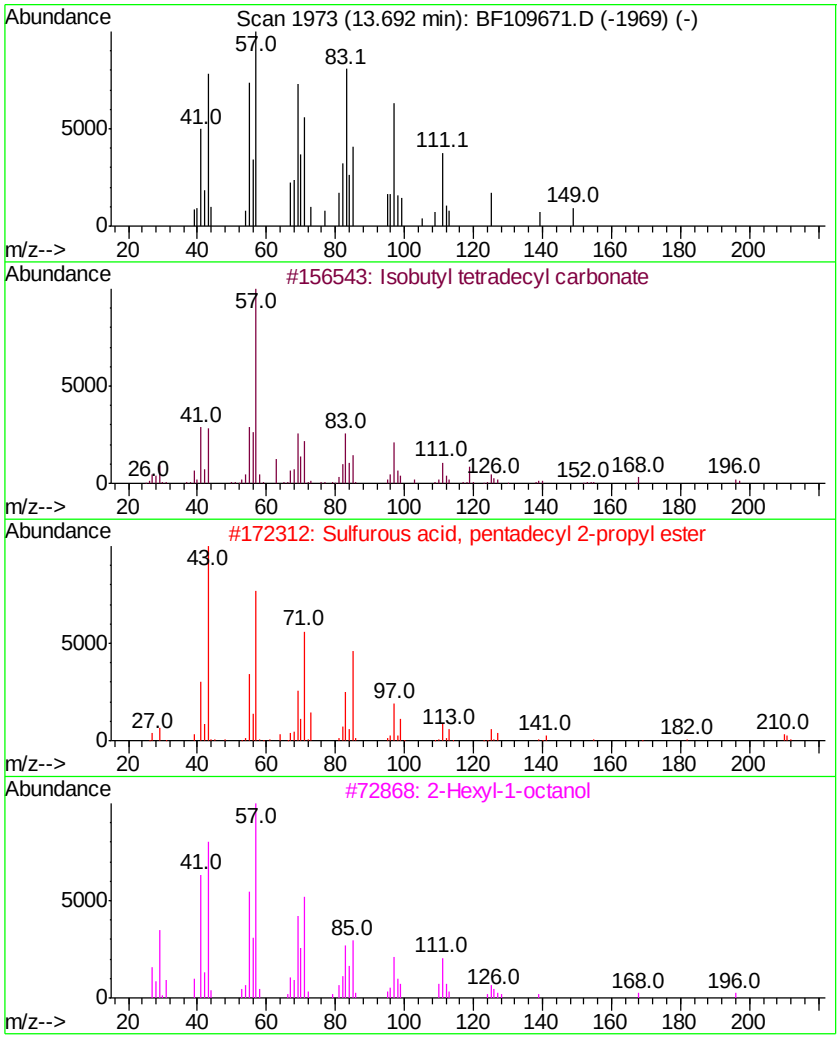
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

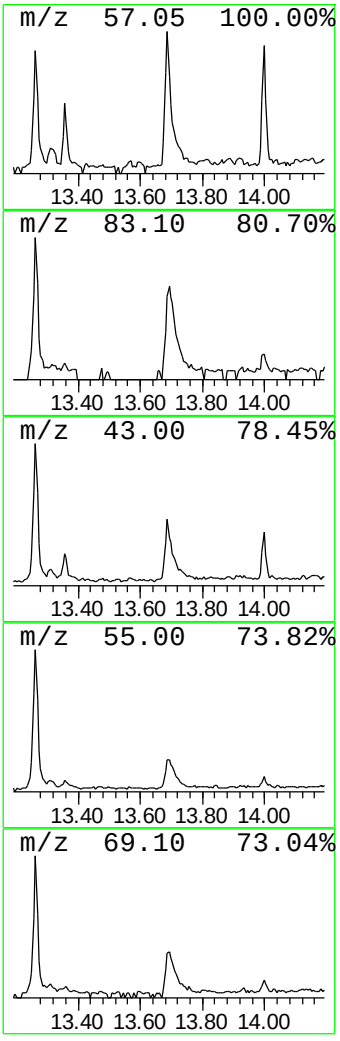
****

Peak Number 6 Isobutyl tetradecyl carbonate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	3.66 ng	110459	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	64
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	59
3	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	53
4	Nonadecane	268	C19H40	000629-92-5	38
5	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

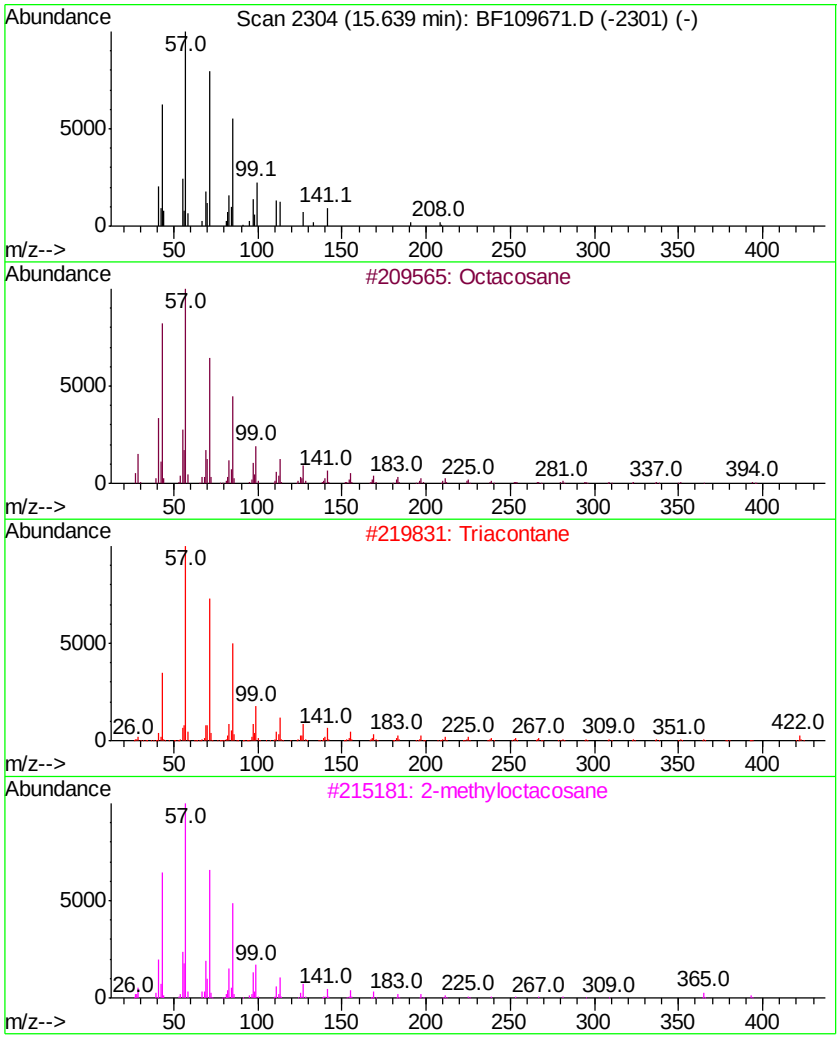
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

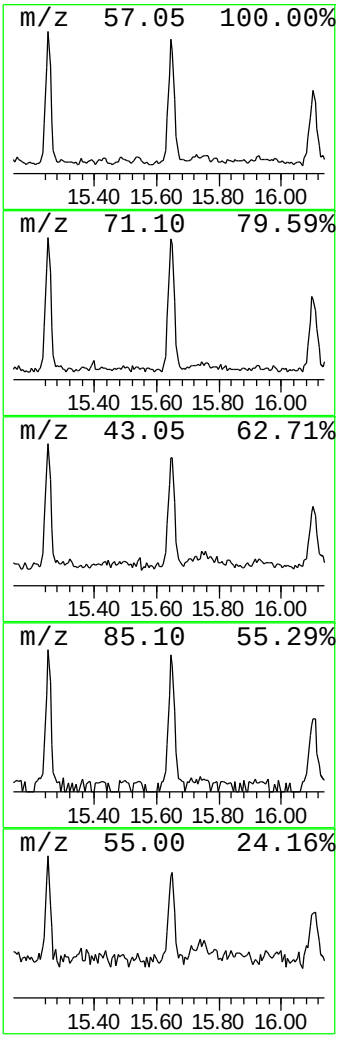
****

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.00 ng	58798	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109671.D
Acq On : 9 Oct 2018 2:09
Operator : JU/SJ
Sample : J5287-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-6

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	2.1	ng	61513	1	6.70	585721	20.0
unknown6.47	6.47	66.8	ng	1955850	1	6.70	585721	20.0
Phenol, 4,4'-(1-m...	12.67	2.6	ng	79479	5	13.83	603691	20.0
9-Octadecenamide,...	13.26	10.4	ng	314217	5	13.83	603691	20.0
Isobutyl tetradec...	13.69	3.7	ng	110459	5	13.83	603691	20.0
Octacosane	15.64	2.0	ng	58798	6	15.22	587634	20.0