LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012319\
Data File : BF112199.D
Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

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-BF011619.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	5.069	499	507	515	rBV	225397	287603	3.67%	0.531%
2	5.487	574	578	592	rBV	4758703	4494219	57.37%	8.298%
3	6.498	745	750	753	rBV	4786469	4787161	61.11%	8.839%
4	6.628	768	772	775	rBV	5482244	5044728	64.40%	9.314%
5	6.851	806	810	817	rBV	1294023	1053153	13.44%	1.945%
6	7.010	833	837	840	rBV	4763880	3996699	51.02%	7.379%
7	7.410	901	905	909	rBV	2980341	3094028	39.50%	5.713%
8	8.134	1024	1028	1045	rBV	1559987	1365446	17.43%	2.521%
9	9.210	1206	1211	1214	rBV	7115842	6354860	81.13%	11.733%
10	9.598	1273	1277	1282	rBV	427186	353431	4.51%	0.653%
11	9.886	1322	1326	1336	rVB2	1771488	1625248	20.75%	3.001%
12	10.680	1457	1461	1474	rBV	4620752	4383213	55.96%	8.093%
13	11.375	1575	1579	1591	rBV	2139656	1833830	23.41%	3.386%
14	11.898	1664	1668	1672	rBV	296206	283438	3.62%	0.523%
15	12.963	1844	1849	1852	rBV	8144993	7833218	100.00%	14.463%
16	13.527	1939	1945	1947	rBV2	69220	78480	1.00%	0.145%
17	13.845	1996	1999	2009	rBV	521876	662235	8.45%	1.223%
18	14.016	2024	2028	2032	rBV	2214641	1989784	25.40%	3.674%
19	14.168	2051	2054	2061	rVB	163787	162767	2.08%	0.301%
20	14.474	2102	2106	2113	rVB	221891	245038	3.13%	0.452%
21	14.780	2155	2158	2162	rVB	261415	241518	3.08%	0.446%
22	14.857	2167	2171	2175	rVV	810466	773040	9.87%	1.427%
23	15.115	2211	2215	2221	rBV	272929	329867	4.21%	0.609%
24	15.492	2273	2279	2285	rBV	1576905	2184309	27.89%	4.033%
25	15.927	2349	2353	2359	rVB	221334	318205	4.06%	0.588%
26	16.433	2434	2439	2448	rVB2	144565	257619	3.29%	0.476%
27	17.027	2535	2540	2546	rVB3	63466	127065	1.62%	0.235%

Sum of corrected areas: 54160202

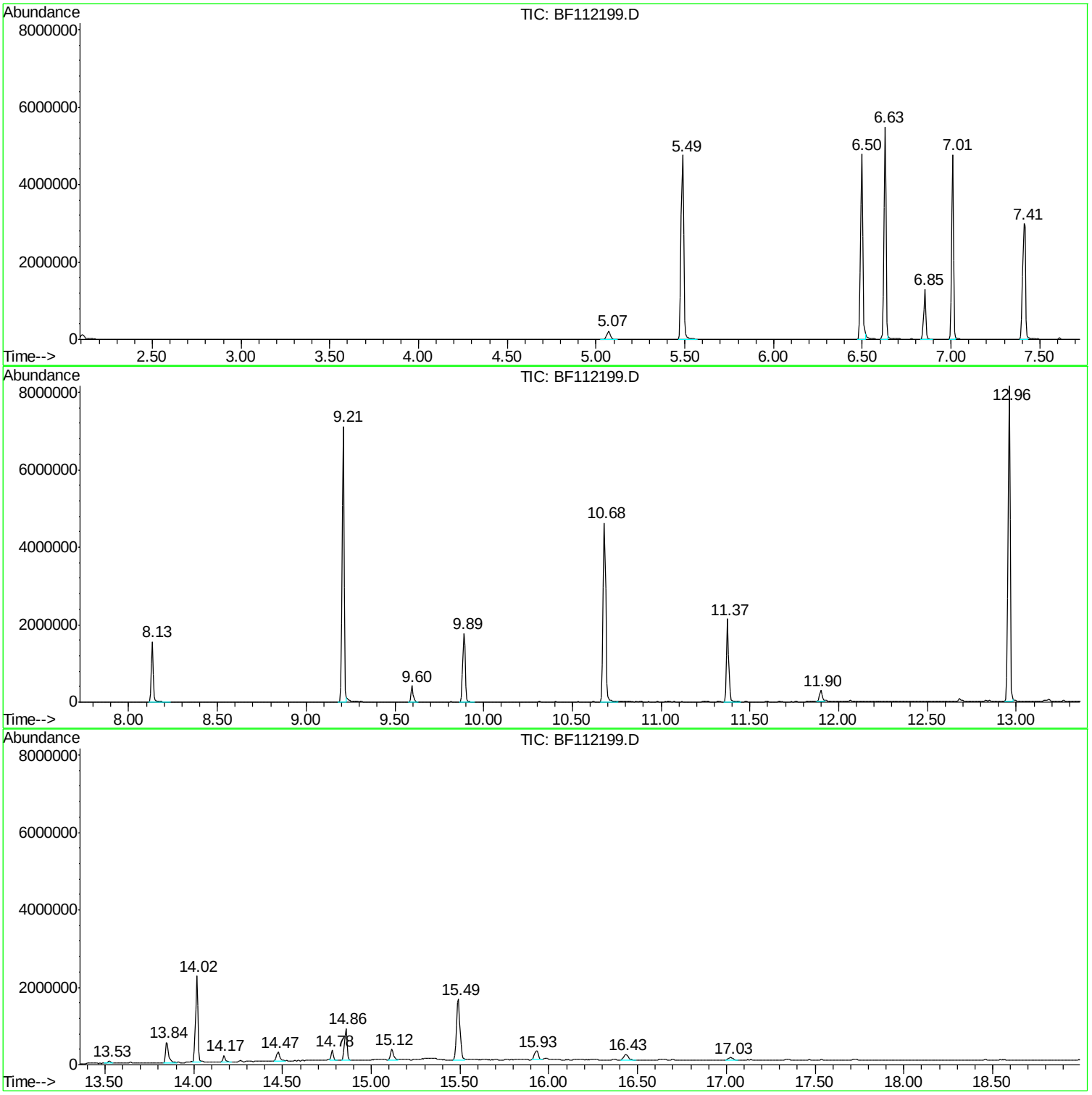
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012319\
Data File : BF112199.D
Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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

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Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : S-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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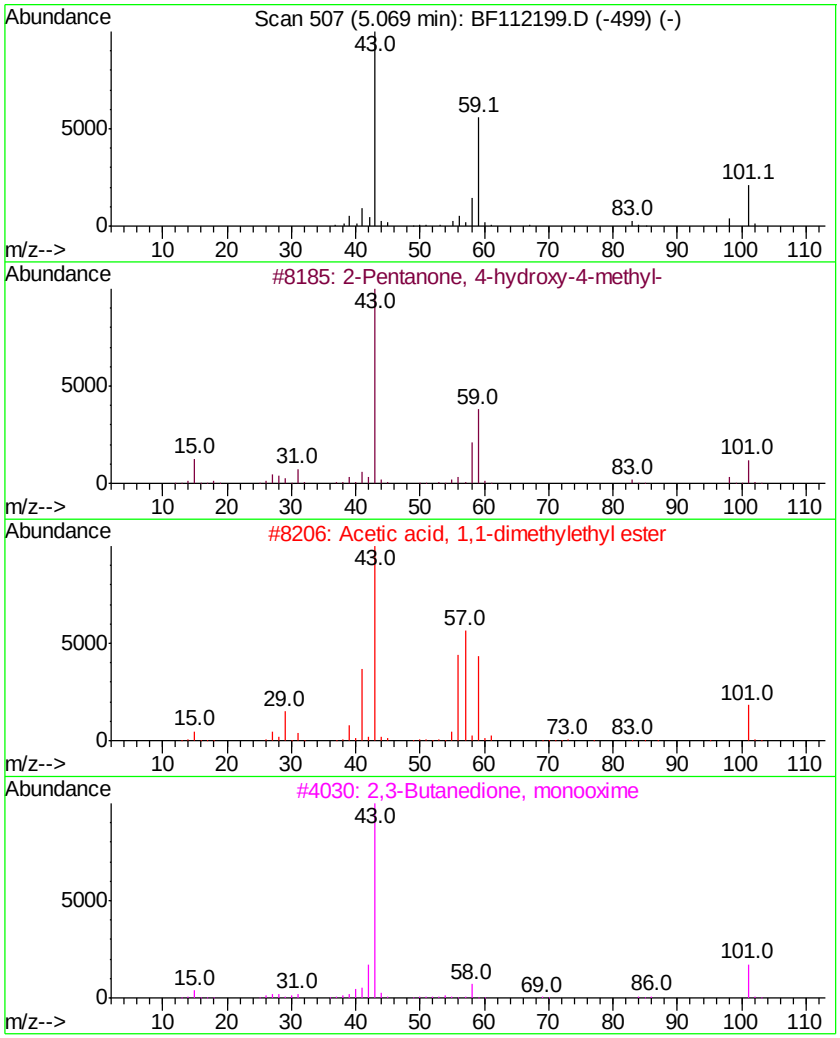
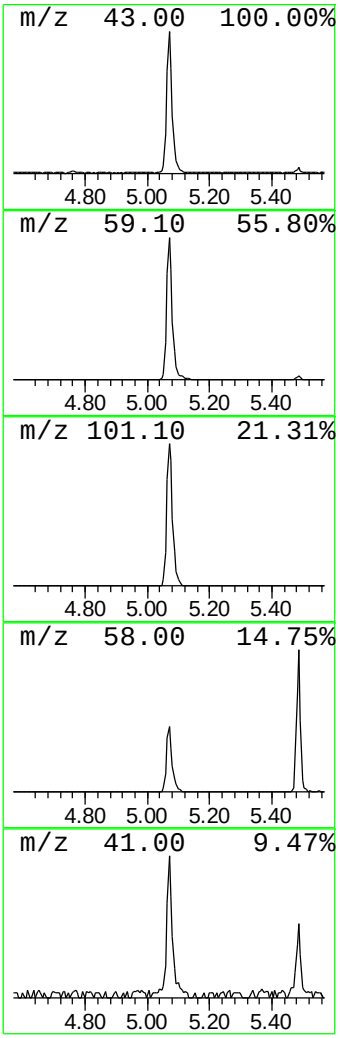
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	5.46 ng	287603	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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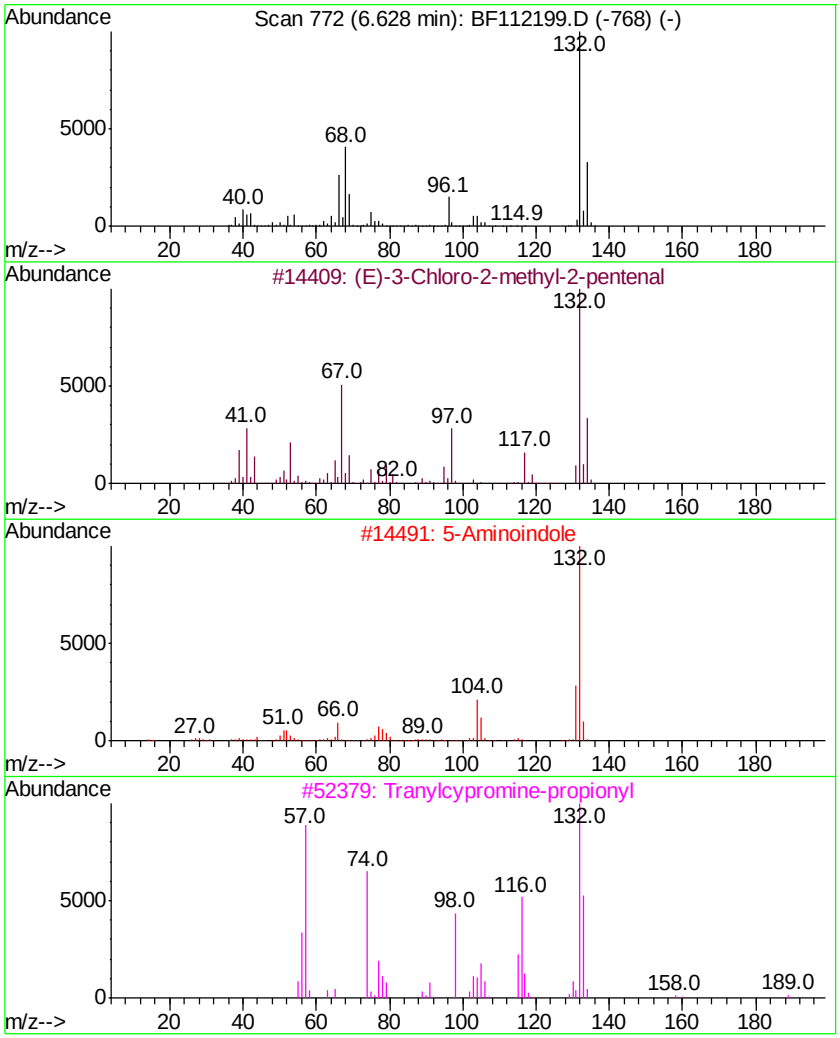
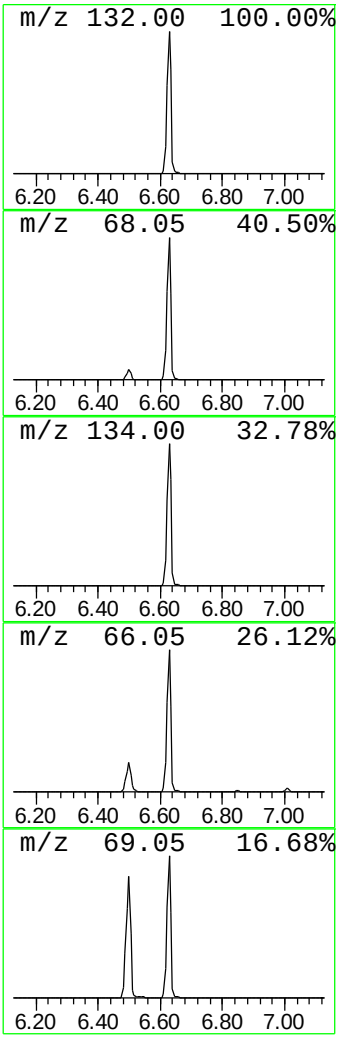
Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	95.80 ng	5044730	1,4-Dichlorobenzene-d4	6.85

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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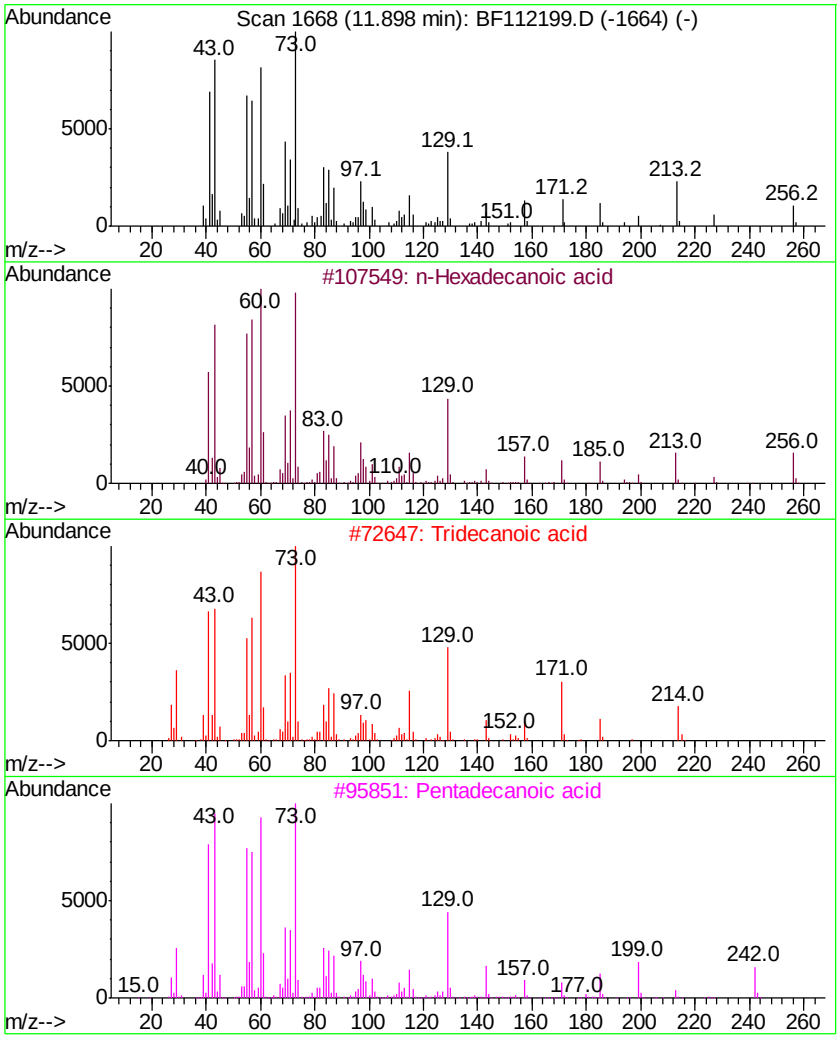
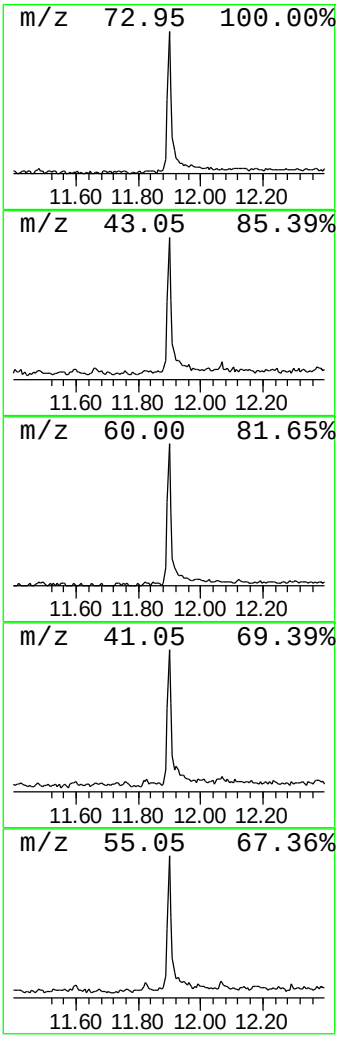
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.09 ng	283438	Phenanthrene-d10	11.37

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

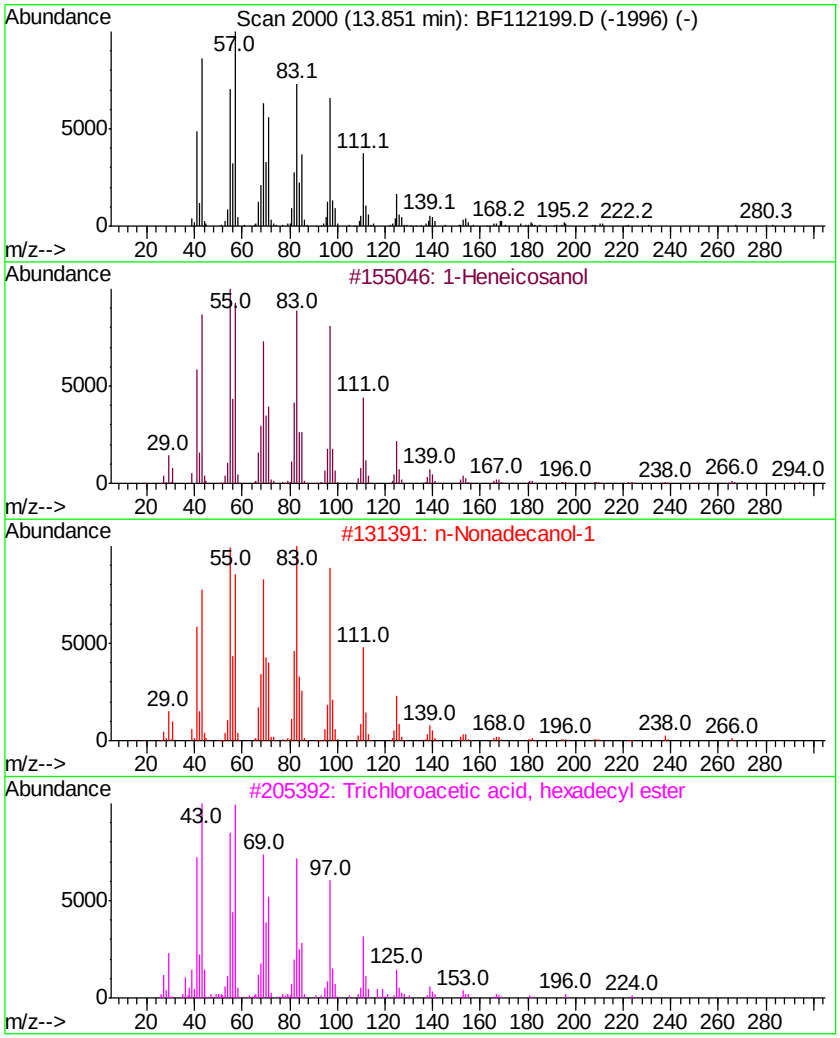
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

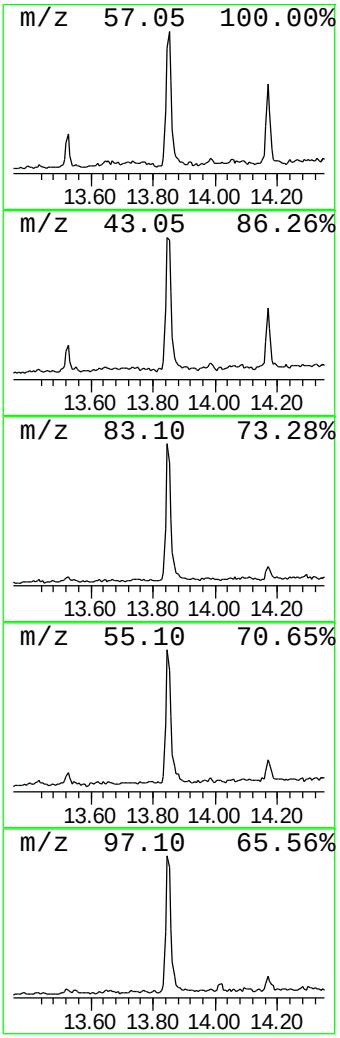
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	6.66 ng	662235	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012319\
Data File : BF112199.D
Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

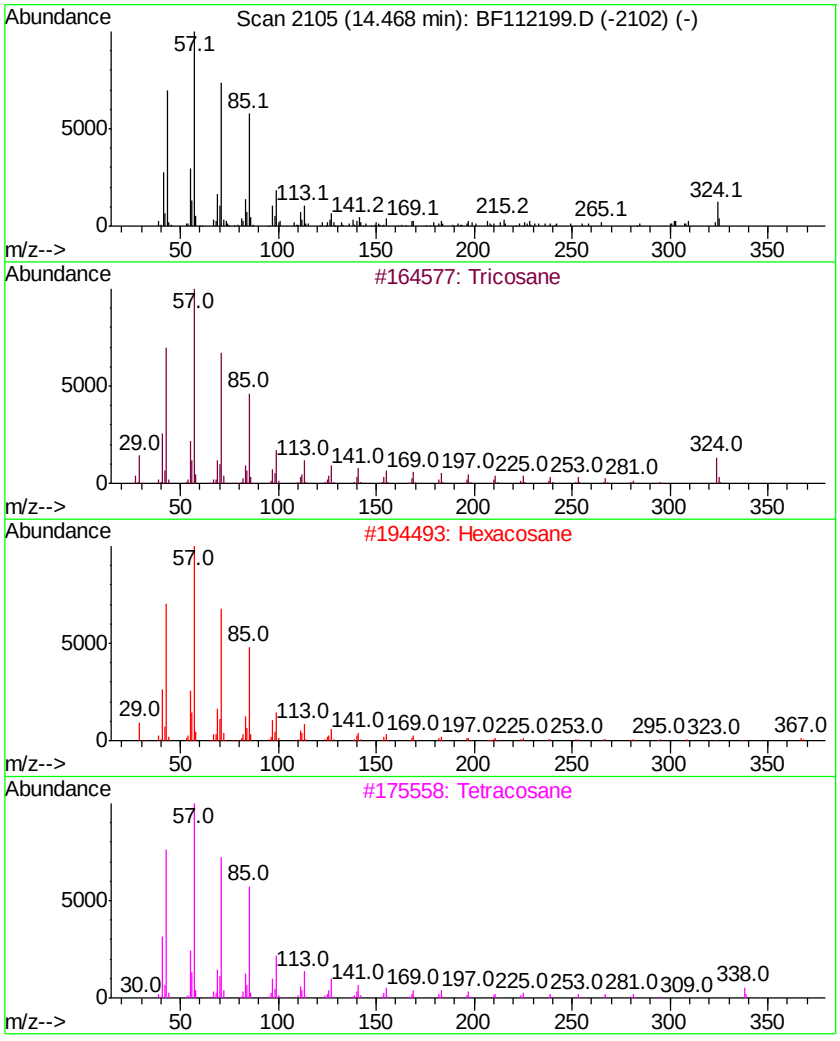
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

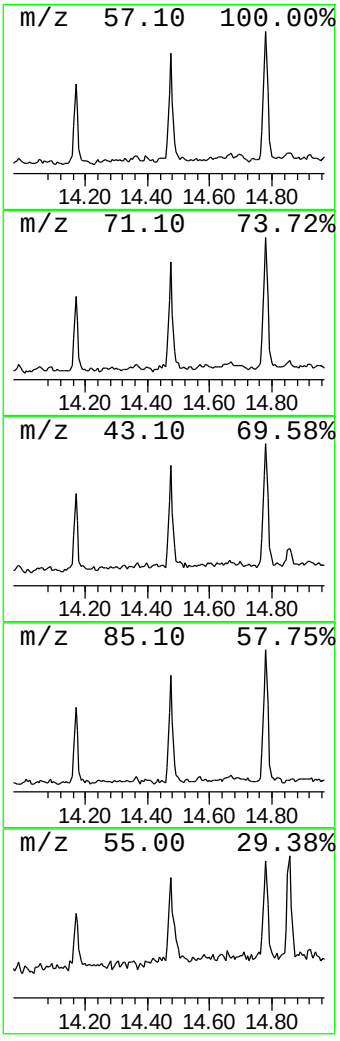
****

Peak Number 6 Tricosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.46 ng	245038	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012319\
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Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

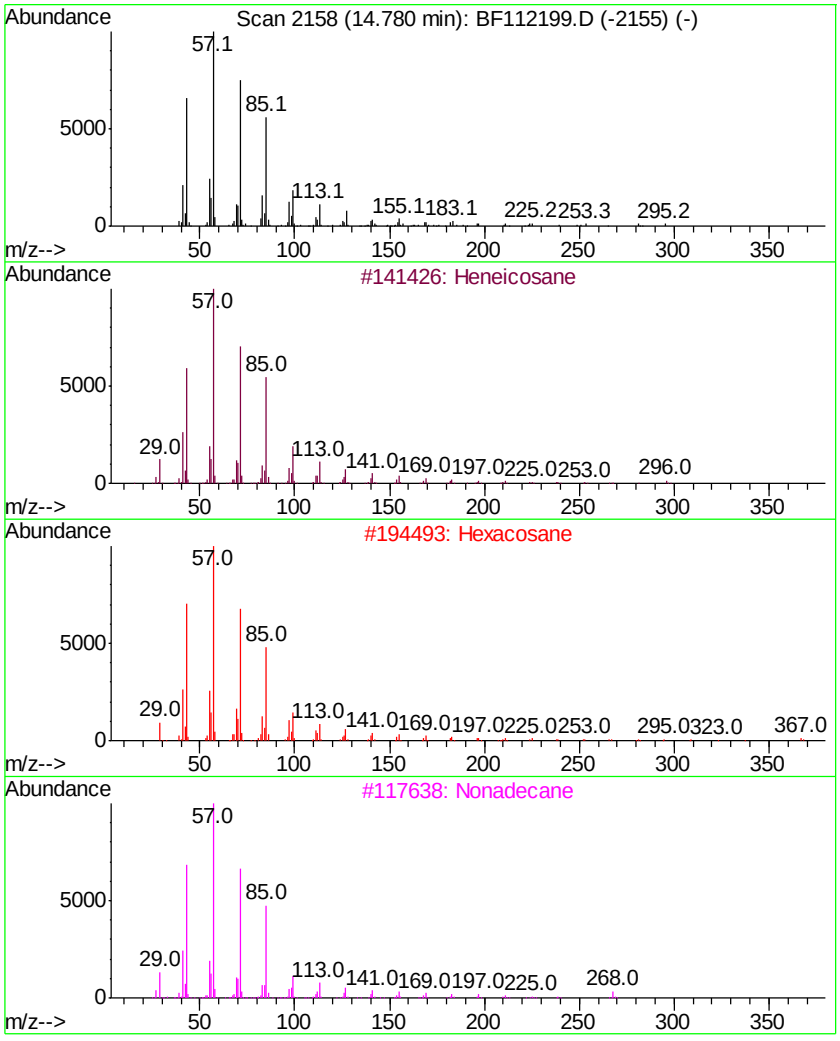
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

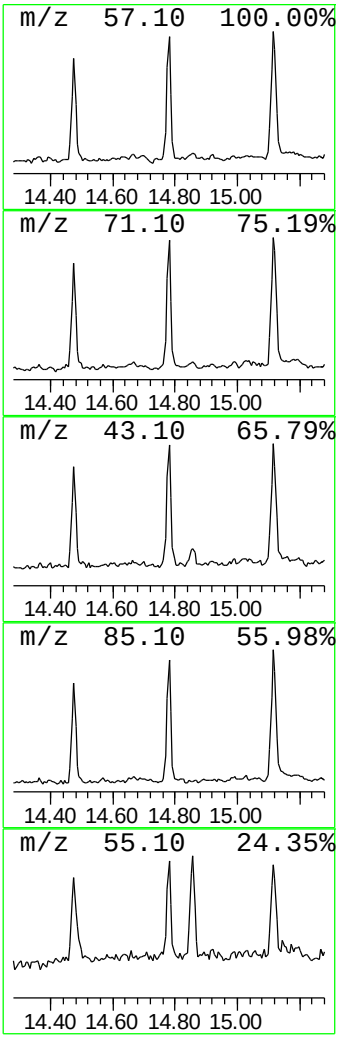
****

Peak Number 7 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.21 ng	241518	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Nonadecane	268	C19H40	000629-92-5	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Octacosane	394	C28H58	000630-02-4	81





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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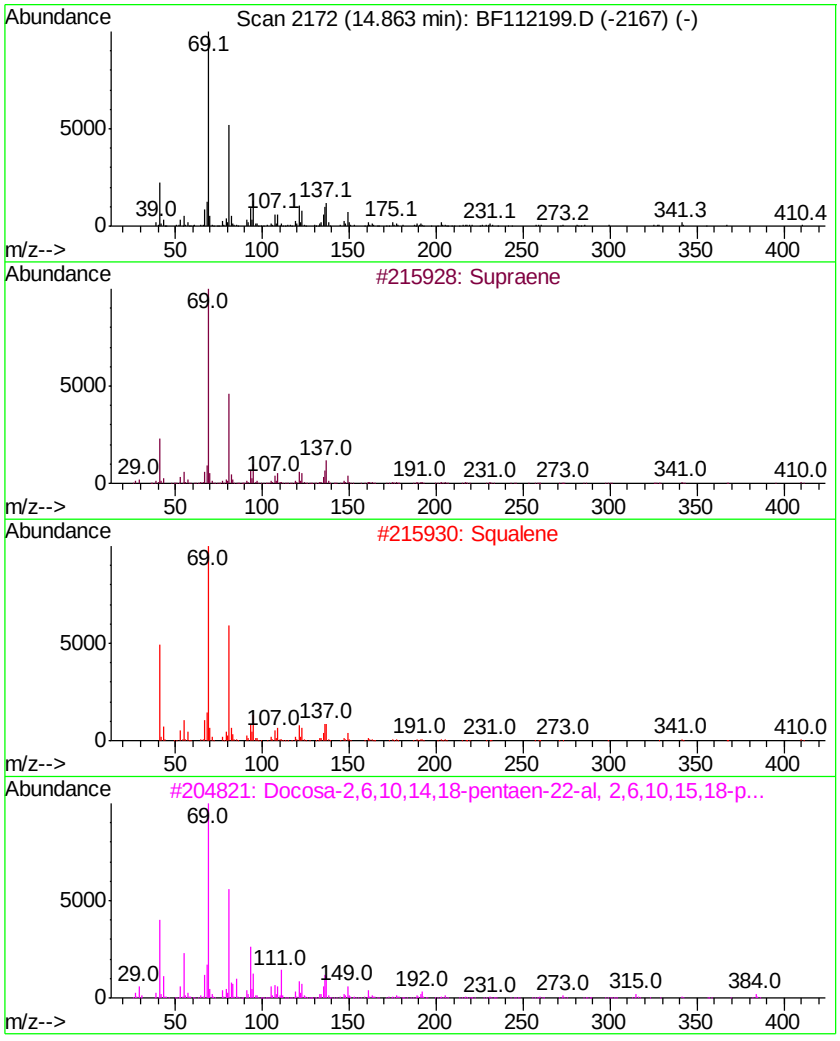
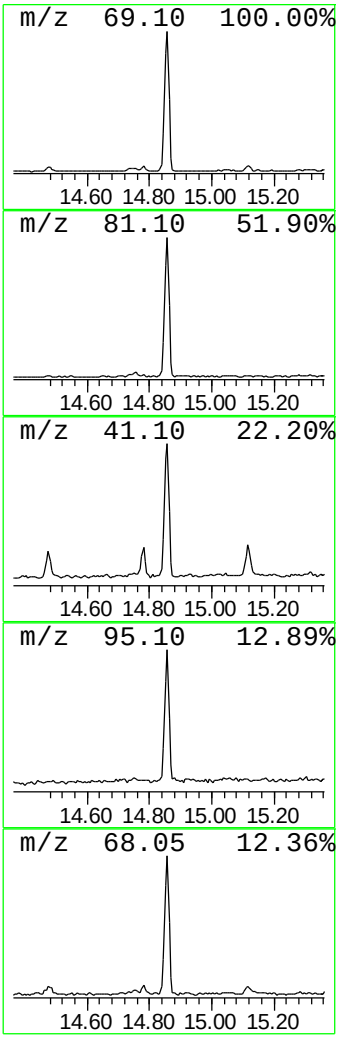
Peak Number 8 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	7.08 ng	773040	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72





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Instrument : BNA_F
ClientSampleId : S-1

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

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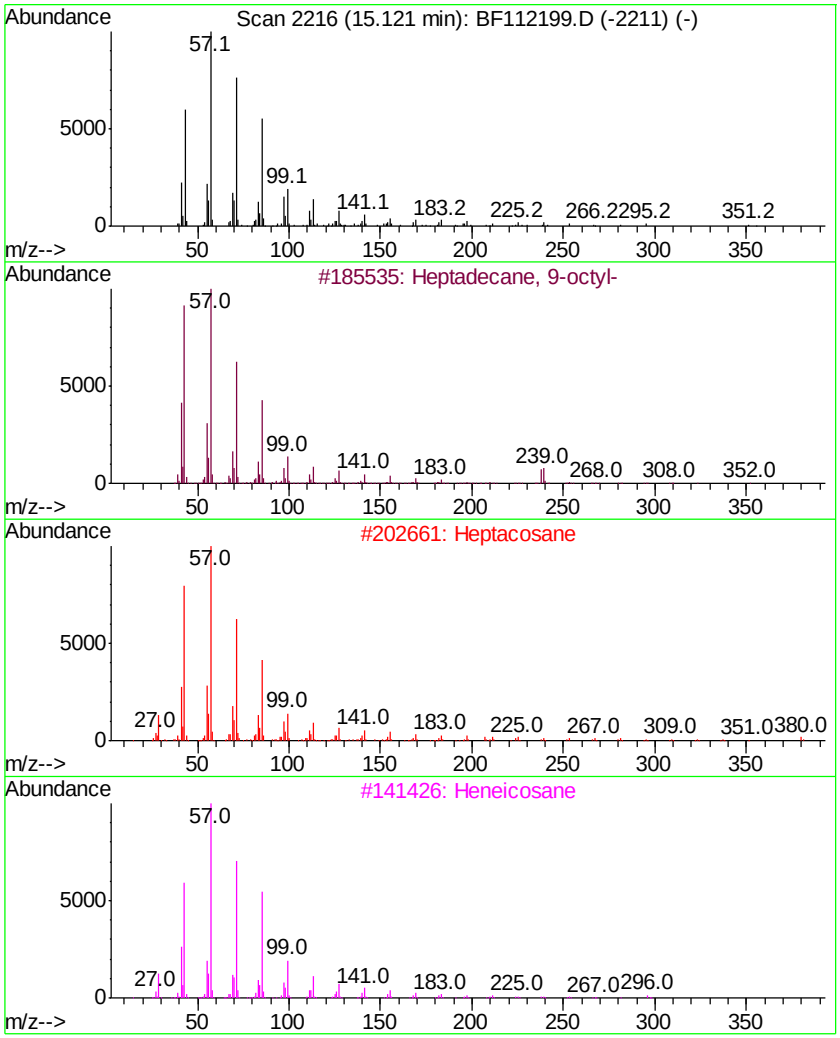
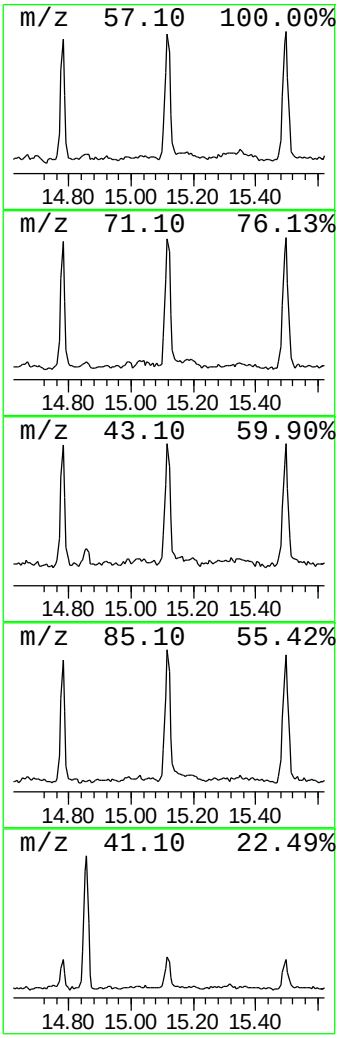
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.02 ng	329867	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Octacosane	394	C28H58	000630-02-4	91





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

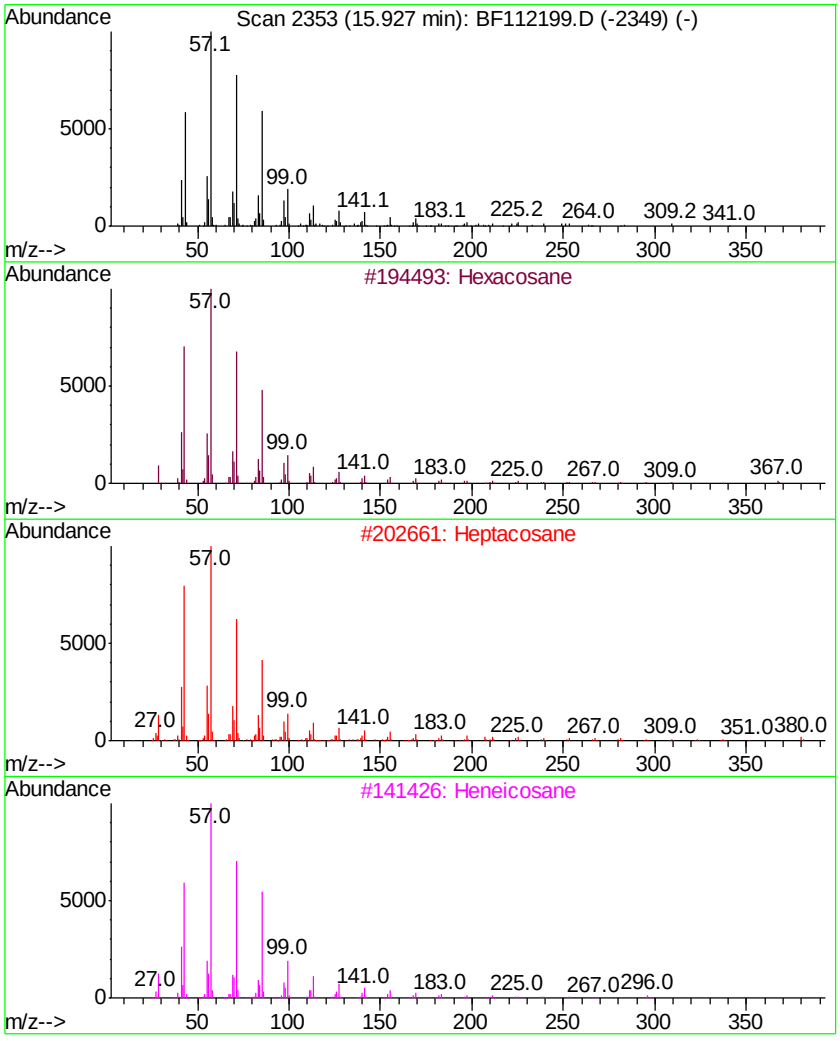
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

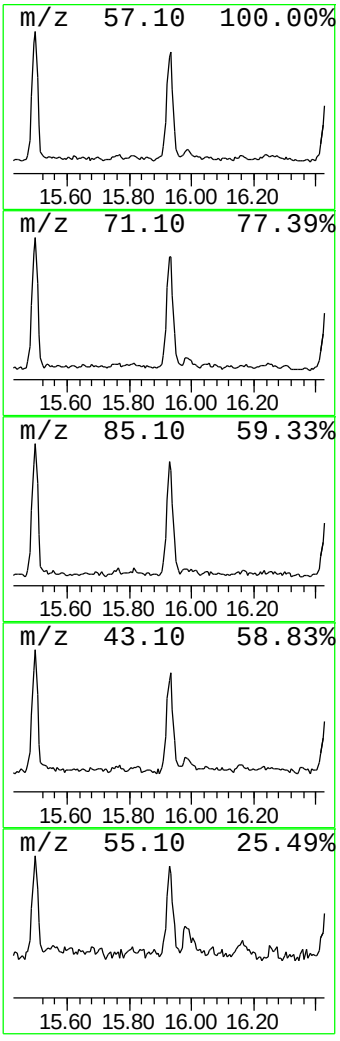
****

Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.91 ng	318205	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012319\
Data File : BF112199.D
Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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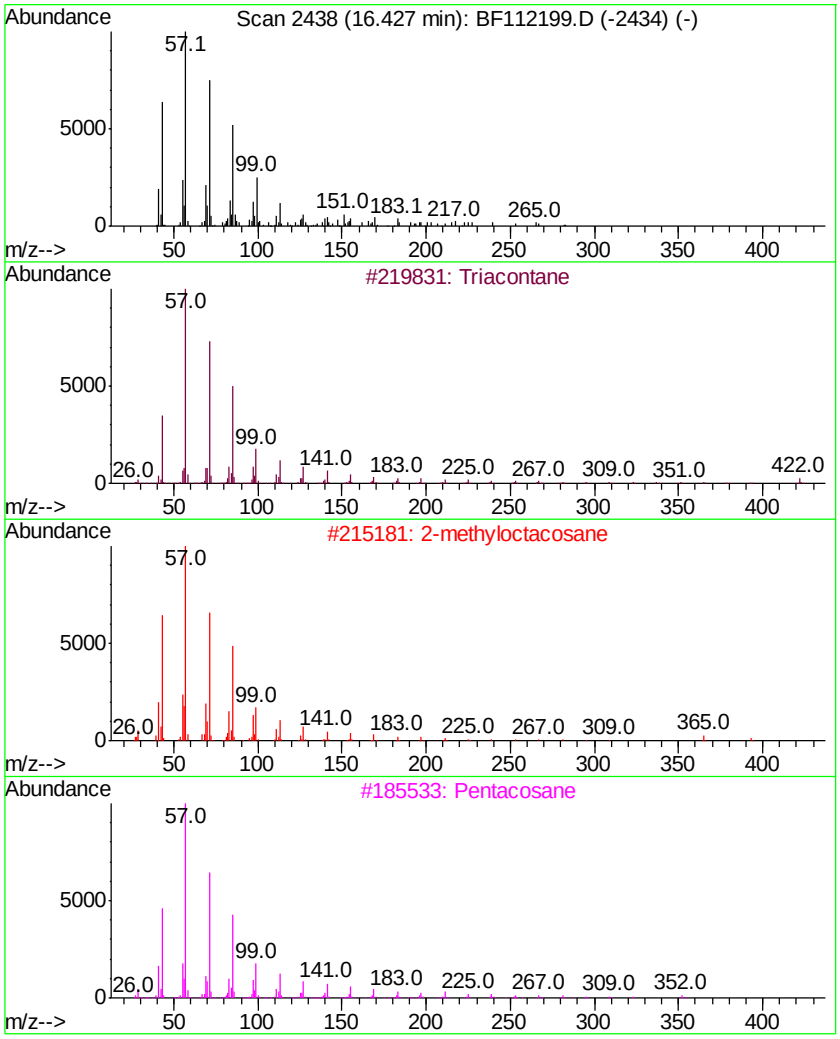
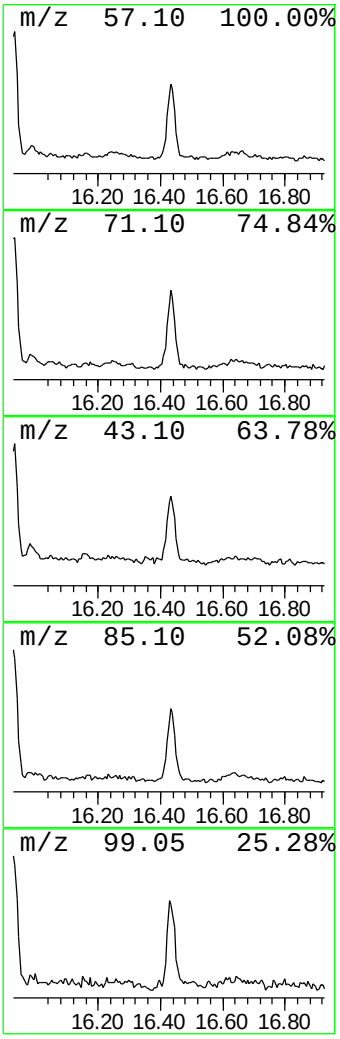
****

Peak Number 11 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.36 ng	257619	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012319\
Data File : BF112199.D
Acq On : 23 Jan 2019 14:02
Operator : JU/SJ
Sample : K1220-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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...	5.07	5.5	ng	287603	1	6.85	1053150	20.0
unknown6.63	6.63	95.8	ng	5044730	1	6.85	1053150	20.0
n-Hexadecanoic acid	11.90	3.1	ng	283438	4	11.37	1833830	20.0
1-Heneicosanol	13.85	6.7	ng	662235	5	14.02	1989780	20.0
Tricosane	14.47	2.5	ng	245038	5	14.02	1989780	20.0
Heneicosane	14.78	2.2	ng	241518	6	15.49	2184310	20.0
Supraene	14.86	7.1	ng	773040	6	15.49	2184310	20.0
Heptadecane, 9-oc...	15.12	3.0	ng	329867	6	15.49	2184310	20.0
Hexacosane	15.93	2.9	ng	318205	6	15.49	2184310	20.0
Triacontane	16.43	2.4	ng	257619	6	15.49	2184310	20.0