LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
Data File : BF116671.D
Acq On : 31 Aug 2019 1:03
Operator : HP/JU
Sample : K4613-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10-S

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-BF083019.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	5.463	569	574	577	rBV	2984958	3146335	79.87%	10.087%
2	6.475	740	746	750	rBV	3025133	3559734	90.37%	11.412%
3	6.616	765	770	773	rBV	3357492	3384424	85.91%	10.850%
4	6.845	805	809	812	rBV	754600	568662	14.44%	1.823%
5	7.004	832	836	839	rBV	2864118	2393263	60.75%	7.672%
6	7.404	899	904	907	rBV	2172304	2134605	54.19%	6.843%
7	8.128	1023	1027	1030	rBV	885610	732594	18.60%	2.349%
8	9.204	1205	1210	1213	rBV	4162160	3613260	91.72%	11.583%
9	9.592	1272	1276	1279	rBV	294413	253533	6.44%	0.813%
10	9.880	1321	1325	1328	rBV	1000303	847945	21.53%	2.718%
11	10.663	1454	1458	1462	rBV	2075819	2184513	55.45%	7.003%
12	11.357	1573	1576	1580	rBV	1008965	877193	22.27%	2.812%
13	11.886	1662	1666	1670	rBV	224287	204011	5.18%	0.654%
14	12.668	1796	1799	1806	rBV	65607	68214	1.73%	0.219%
15	12.945	1841	1846	1849	rBV	3693279	3939275	100.00%	12.629%
16	13.521	1941	1944	1946	rVB	54151	44137	1.12%	0.141%
17	13.833	1994	1997	2014	rBV2	435270	528264	13.41%	1.694%
18	13.986	2020	2023	2027	rVB	877592	823389	20.90%	2.640%
19	14.162	2048	2053	2057	rBV	109114	107870	2.74%	0.346%
20	14.468	2099	2105	2119	rBV	184533	227851	5.78%	0.730%
21	14.768	2152	2156	2166	rBV	113419	134342	3.41%	0.431%
22	14.845	2166	2169	2173	rVB	84238	82567	2.10%	0.265%
23	15.104	2209	2213	2222	rBV	112830	165994	4.21%	0.532%
24	15.445	2265	2271	2274	rBV	640740	794487	20.17%	2.547%
25	15.480	2274	2277	2286	rVB	92184	125476	3.19%	0.402%
26	15.915	2345	2351	2355	rBV2	83348	122192	3.10%	0.392%
27	15.956	2355	2358	2364	rVV5	37891	69203	1.76%	0.222%
28	16.409	2431	2435	2441	rVB4	36009	59884	1.52%	0.192%

Sum of corrected areas: 31193217

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
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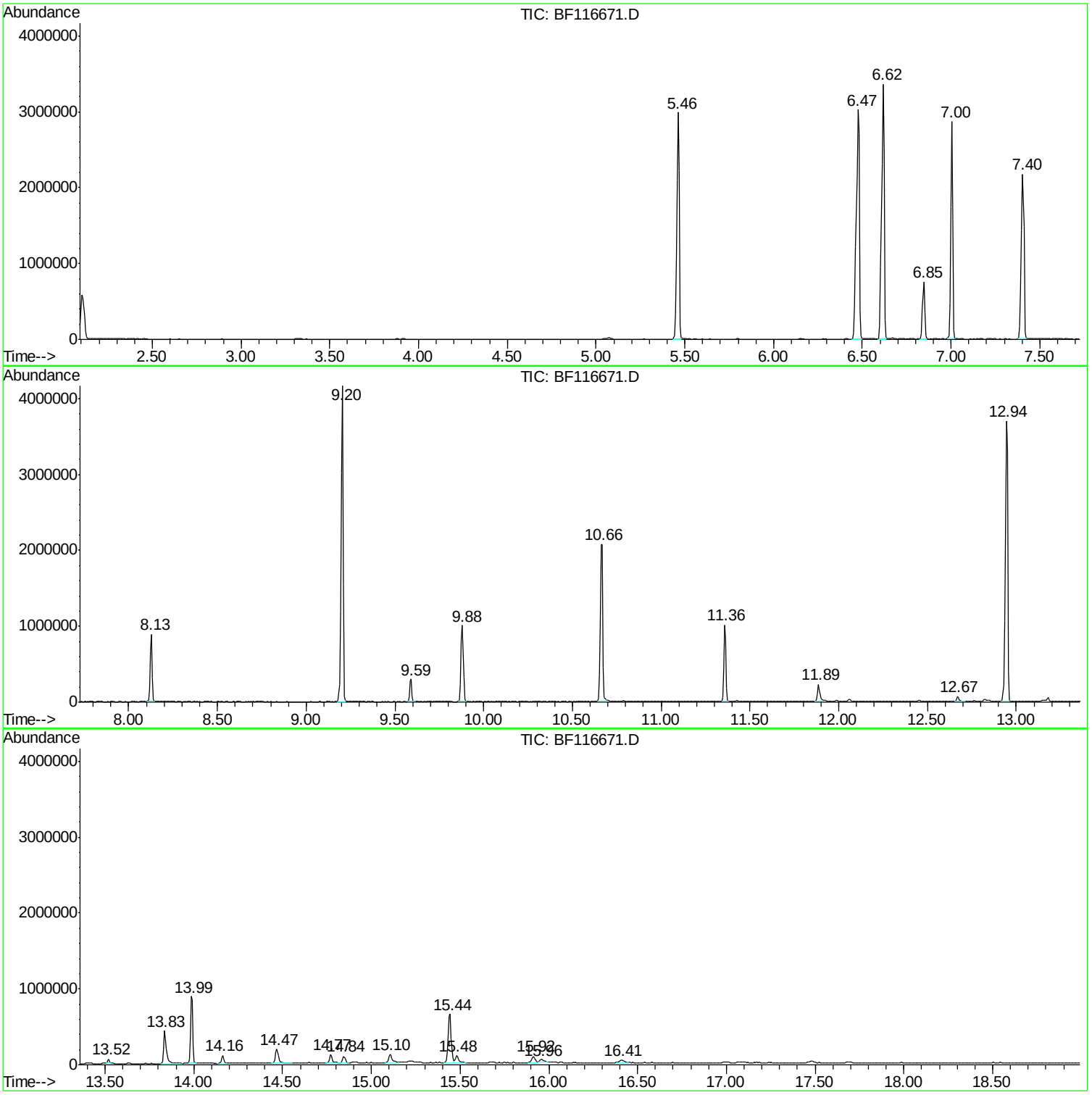
Acq On : 31 Aug 2019 1:03
Operator : HP/JU
Sample : K4613-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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Data File : BF116671.D
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Operator : HP/JU
Sample : K4613-03
Misc :
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Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

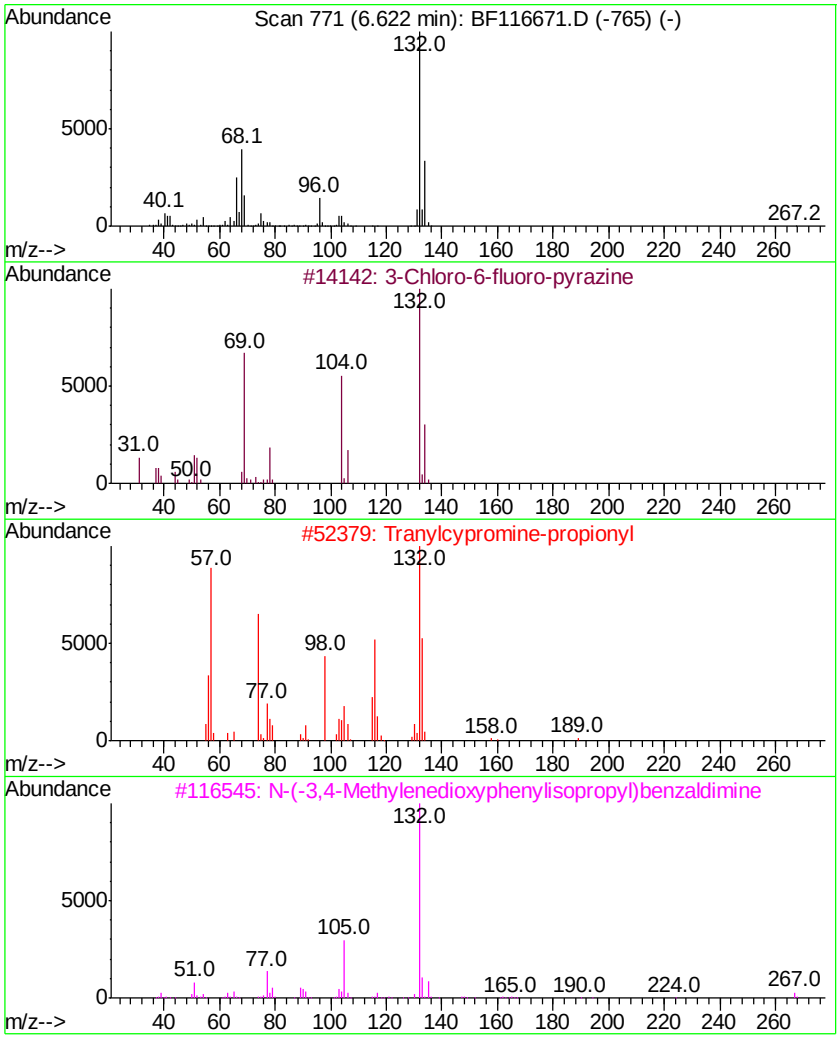
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

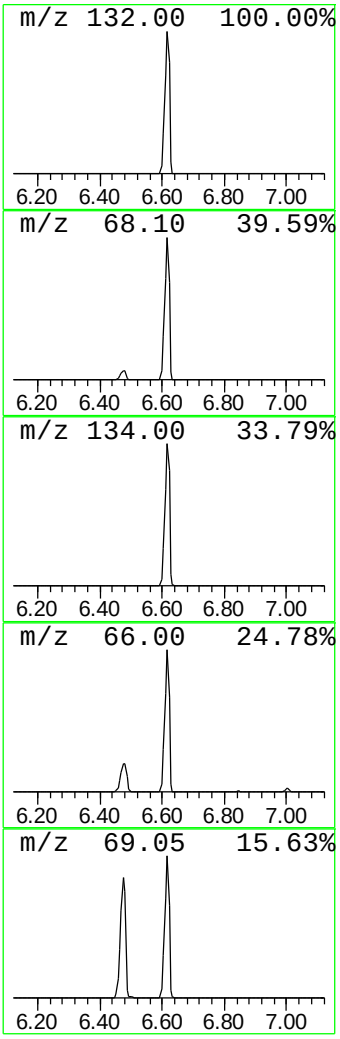
****

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	119.03 ng	3384420	1,4-Dichlorobenzene-d4	6.85

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	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

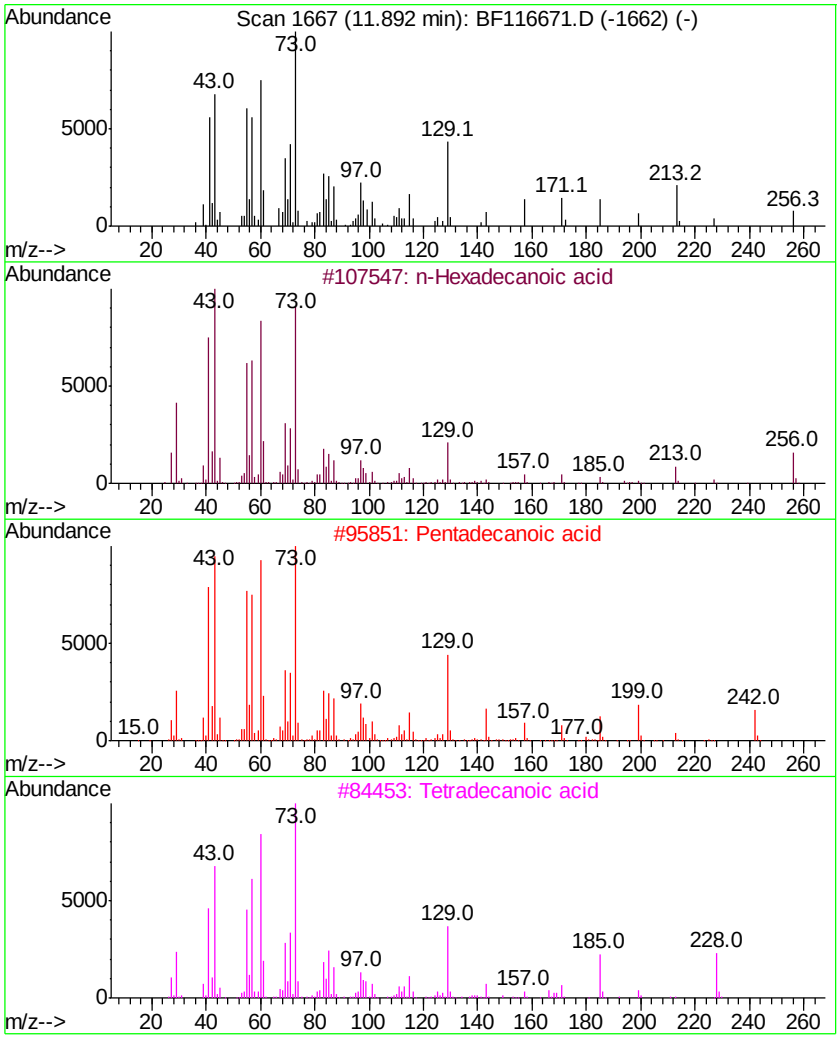
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

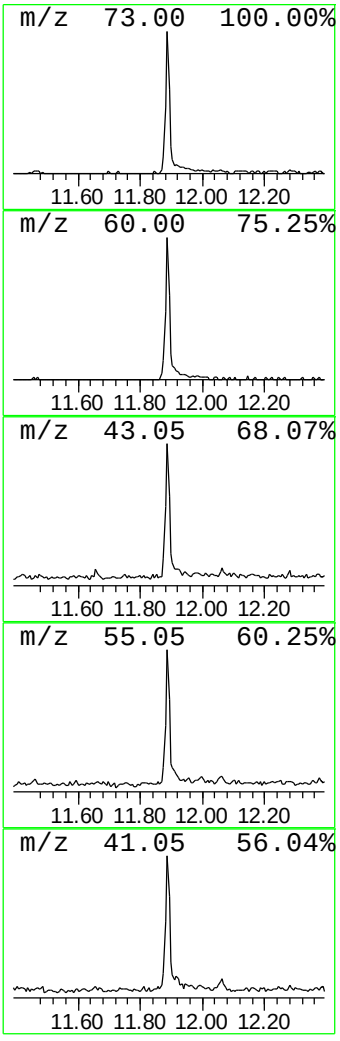
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.65 ng	204011	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Library Search Compound Report

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Data File : BF116671.D
Acq On : 31 Aug 2019 1:03
Operator : HP/JU
Sample : K4613-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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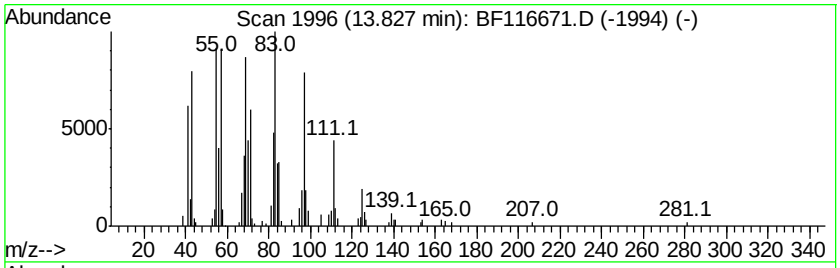
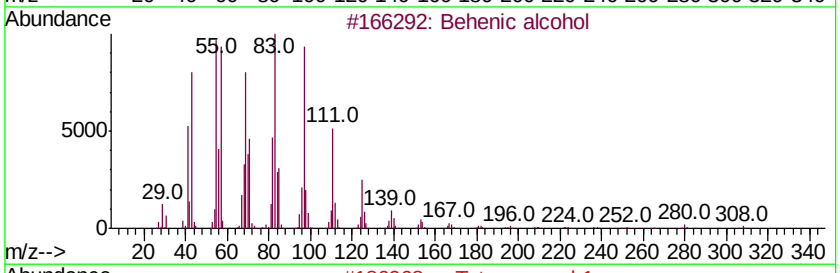
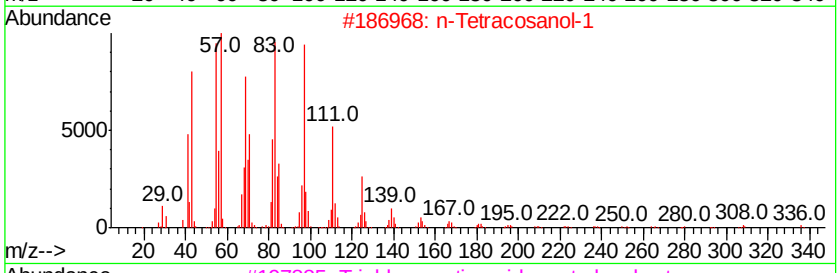
Peak Number 4 Behenic alcohol Concentration Rank 3

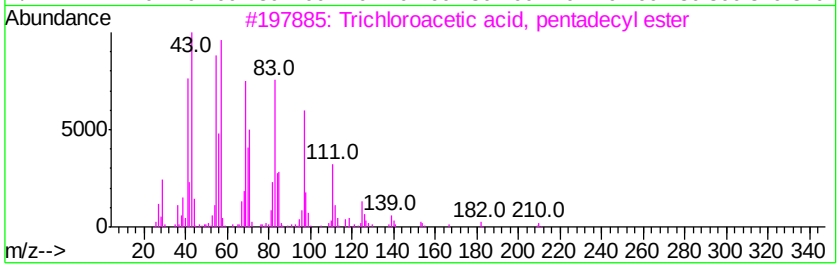
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	12.83 ng	528264	Chrysene-d12	13.99

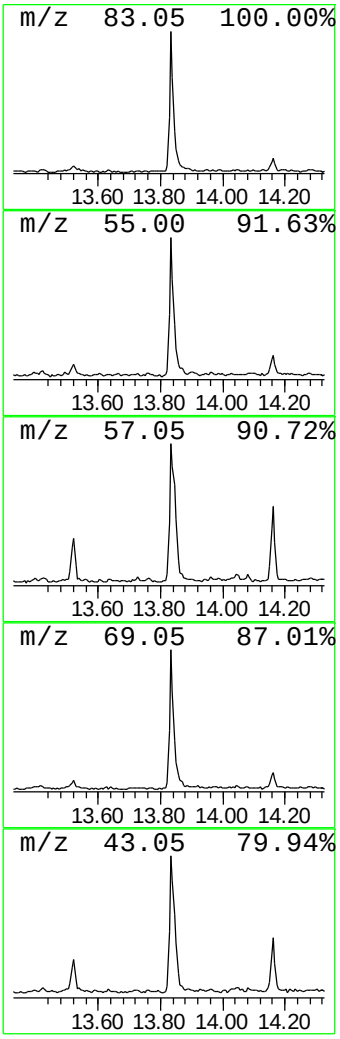
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Isoheptadecanol	256	C17H36O	057289-07-3	90











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Data File : BF116671.D
Acq On : 31 Aug 2019 1:03
Operator : HP/JU
Sample : K4613-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

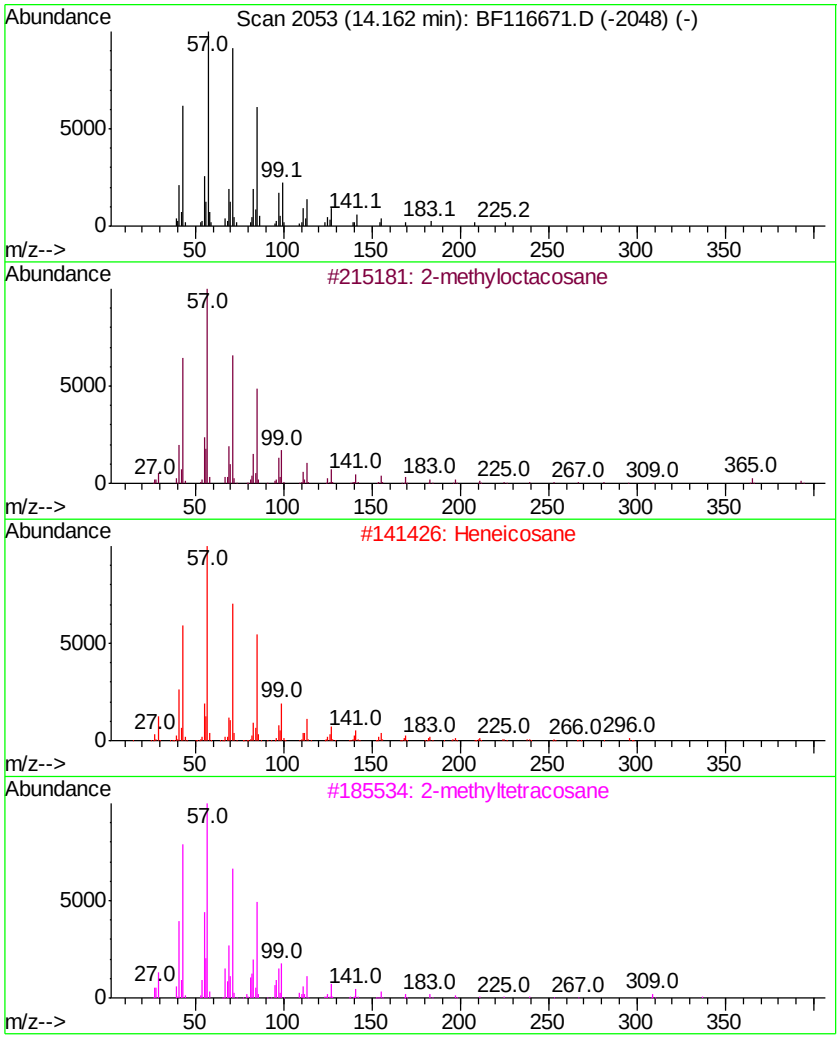
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

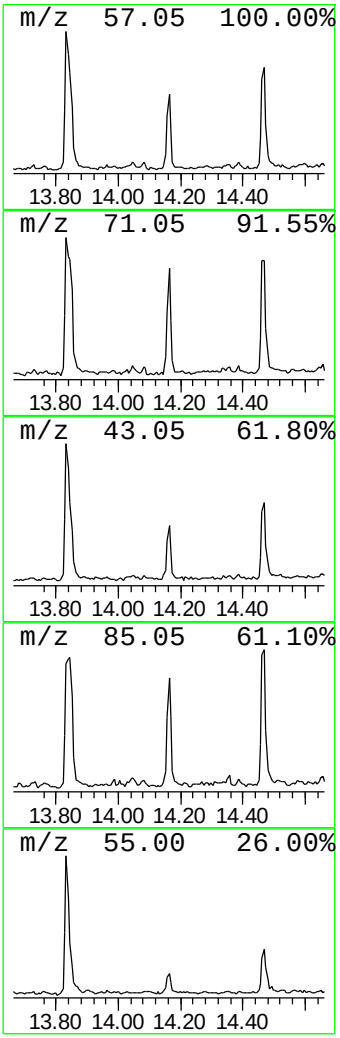
****

Peak Number 5 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	2.62 ng	107870	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyltetracosane	352	C25H52	1000376-72-6	90
4	Octacosane	394	C28H58	000630-02-4	86
5	Tetratetracontane	619	C44H90	007098-22-8	83





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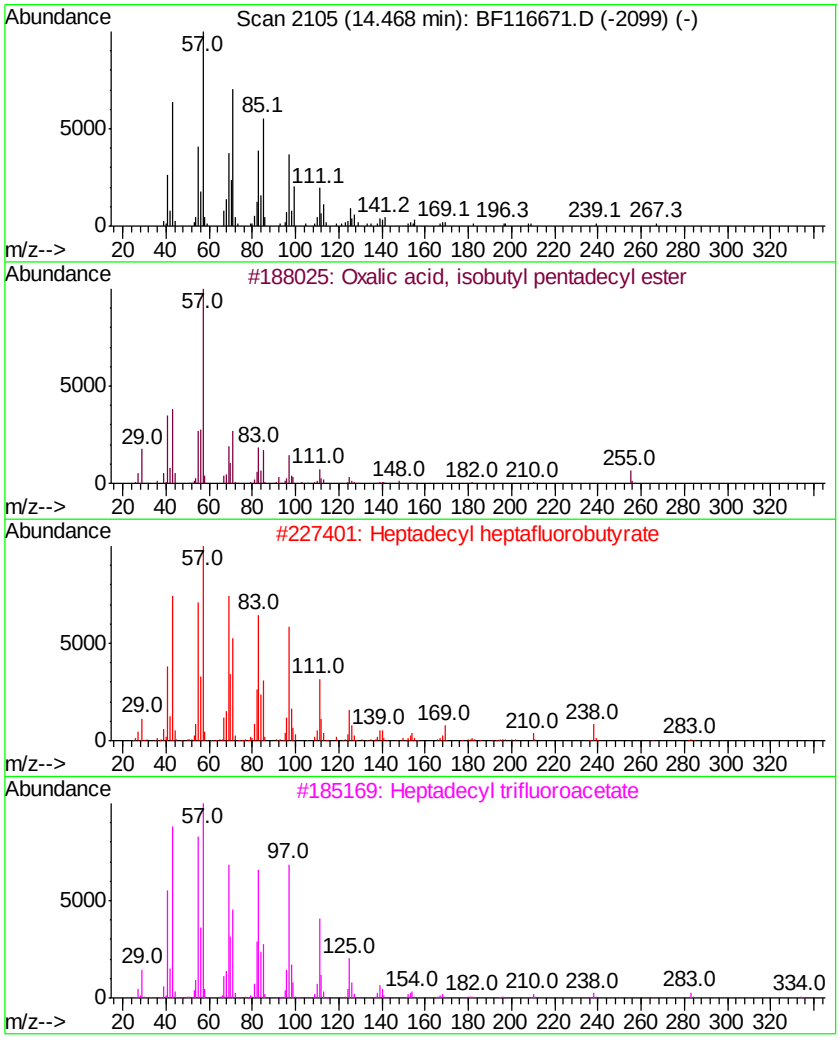
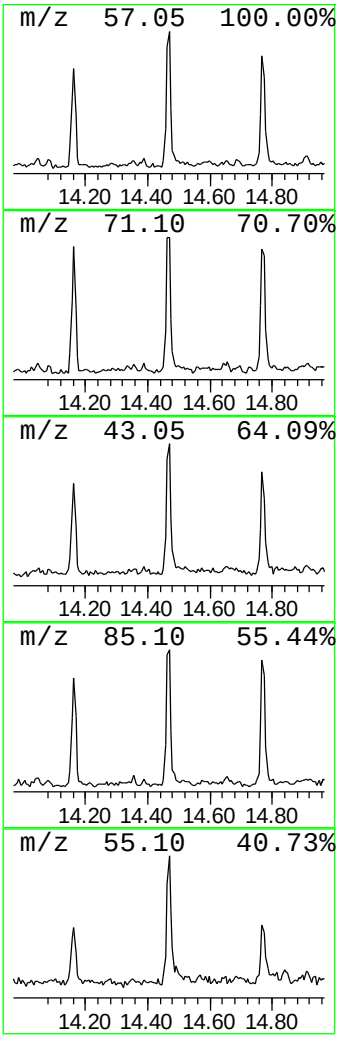
****

Peak Number 6 Oxalic acid, isobutyl penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	5.53 ng	227851	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	72
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	53
4	Tritetracontane	605	C43H88	007098-21-7	52
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	49





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-10-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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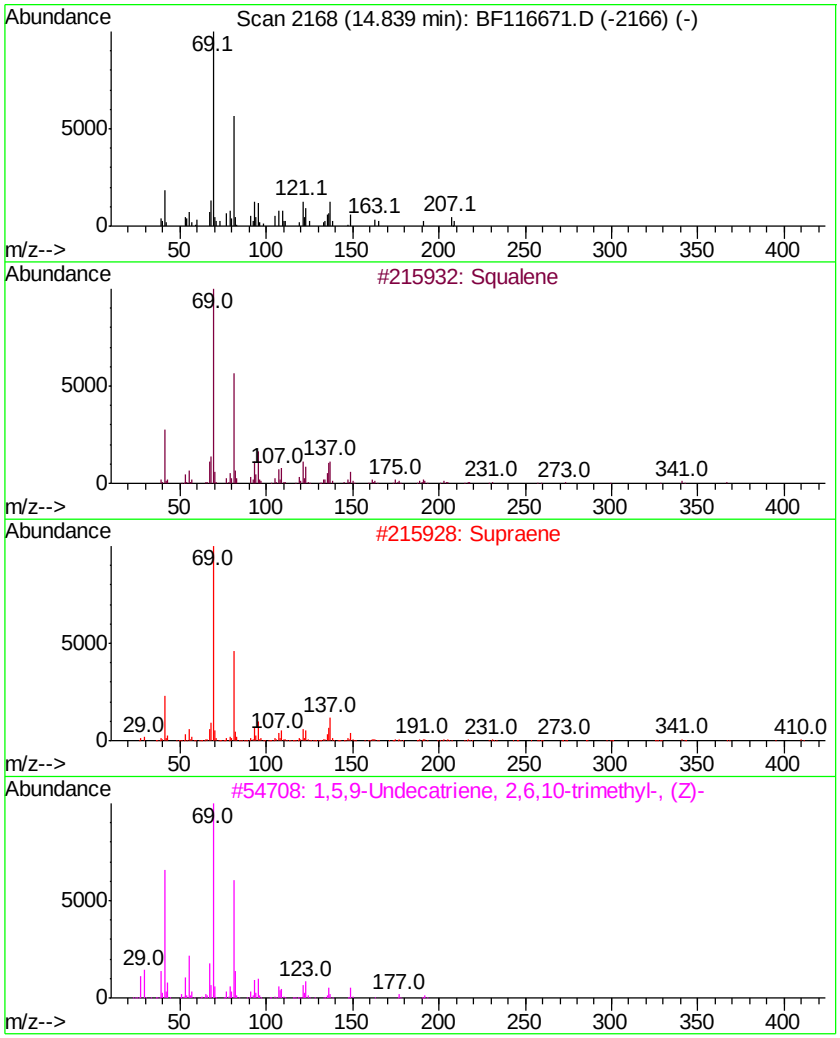
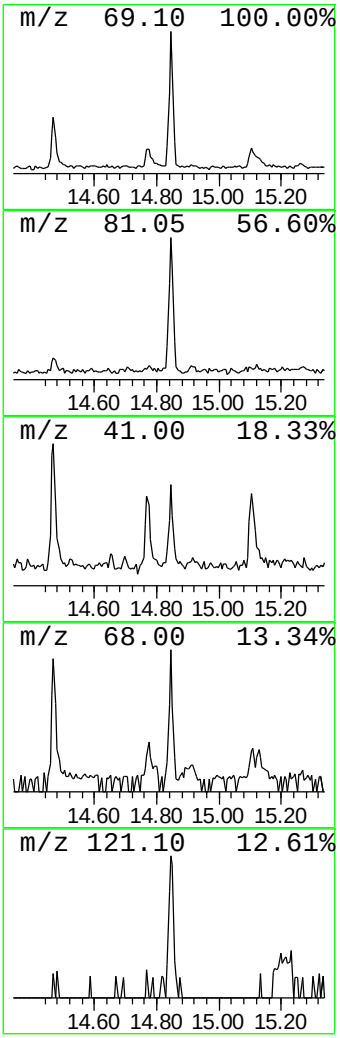
****

Peak Number 8 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.08 ng	82567	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83





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Sample : K4613-03
Misc :
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Instrument : BNA_F
ClientSampleId : TP-10-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

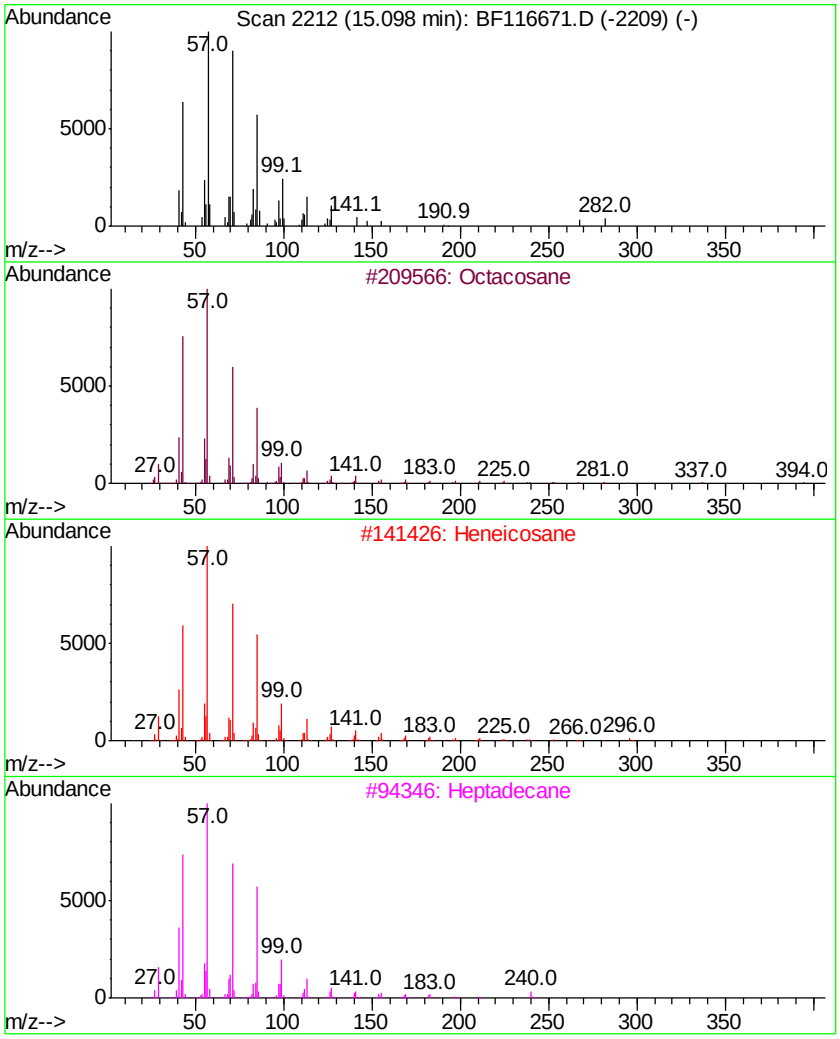
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

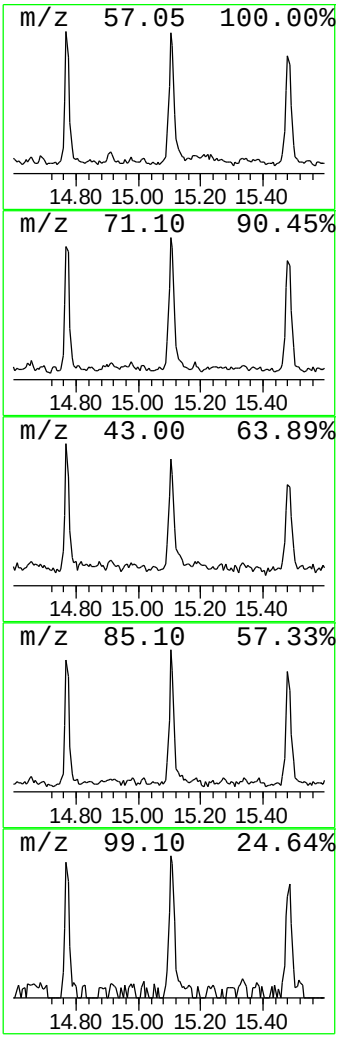
****

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	4.18 ng	165994	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	87
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5	Octadecane	254	C18H38	000593-45-3	86





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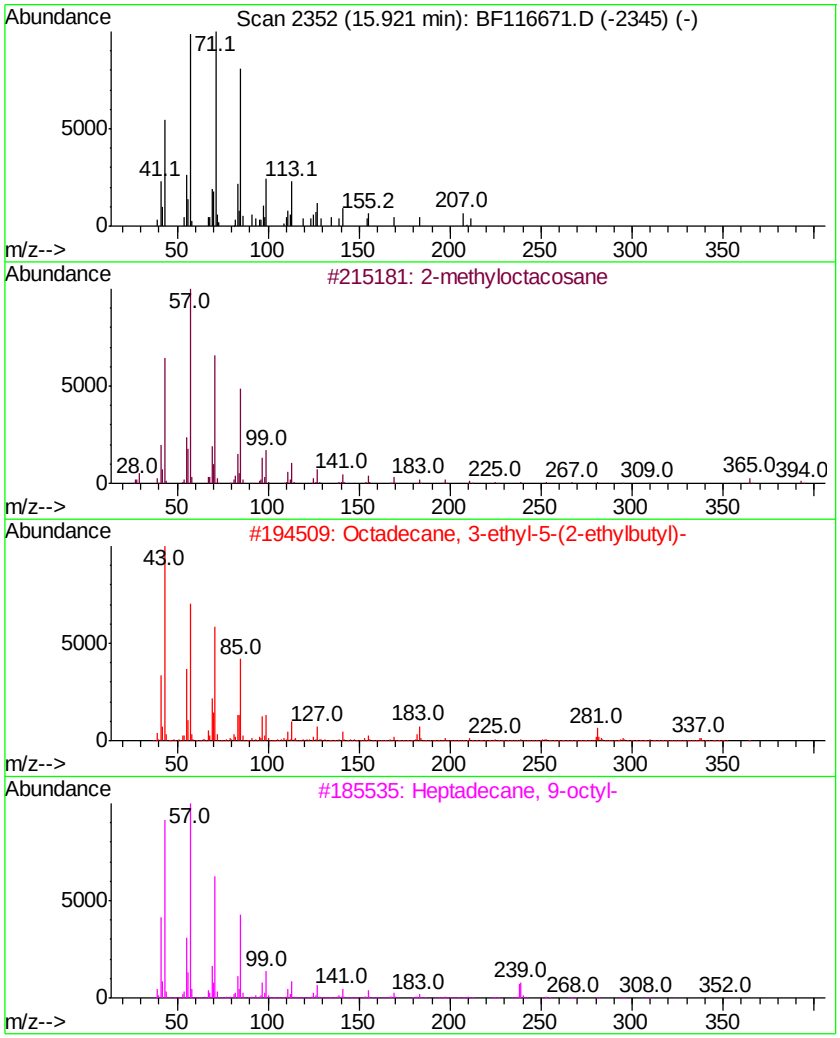
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

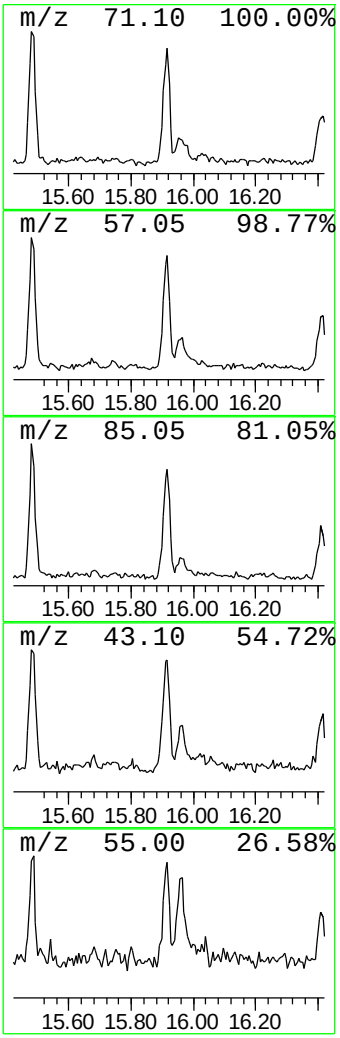
****

Peak Number 10 Octadecane, 3-ethyl-5-(2-et... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.08 ng	122192	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083019\
Data File : BF116671.D
Acq On : 31 Aug 2019 1:03
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Sample : K4613-03
Misc :
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Instrument : BNA_F
ClientSampleId : TP-10-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.62	6.62	119.0	ng	3384420	1	6.85	568662	20.0
n-Hexadecanoic acid	11.89	4.7	ng	204011	4	11.36	877193	20.0
Behenic alcohol	13.83	12.8	ng	528264	5	13.99	823389	20.0
2-methyloctacosane	14.16	2.6	ng	107870	5	13.99	823389	20.0
Oxalic acid, isob...	14.47	5.5	ng	227851	5	13.99	823389	20.0
Squalene	14.84	2.1	ng	82567	6	15.44	794487	20.0
Octacosane	15.10	4.2	ng	165994	6	15.44	794487	20.0
Octadecane, 3-eth...	15.92	3.1	ng	122192	6	15.44	794487	20.0