LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118270.D
Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

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-BF120619.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	502	507	517	rVB	371299	476283	14.34%	1.765%
2	5.481	572	577	594	rBV	2653421	2585493	77.87%	9.582%
3	6.492	744	749	752	rBV	2573476	2664558	80.25%	9.875%
4	6.634	768	773	776	rBV	3270021	2907676	87.57%	10.776%
5	6.857	808	811	820	rBV	698692	564415	17.00%	2.092%
6	7.016	834	838	841	rBV	2802325	2256333	67.96%	8.362%
7	7.422	903	907	919	rBV	1646879	1695985	51.08%	6.285%
8	8.145	1027	1030	1045	rBV	772433	709366	21.36%	2.629%
9	9.228	1209	1214	1225	rBV	3605351	3320249	100.00%	12.305%
10	9.622	1278	1281	1292	rBV	106780	108906	3.28%	0.404%
11	9.910	1326	1330	1342	rBV	893370	830806	25.02%	3.079%
12	10.704	1460	1465	1481	rBV	2258269	2247517	67.69%	8.330%
13	11.404	1580	1584	1593	rBV	789270	814399	24.53%	3.018%
14	11.922	1669	1672	1689	rBV	189855	234437	7.06%	0.869%
15	12.716	1803	1807	1818	rBV	40754	64130	1.93%	0.238%
16	12.992	1850	1854	1857	rBV	3648740	3141703	94.62%	11.643%
17	13.886	2002	2006	2021	rBV	246173	375306	11.30%	1.391%
18	14.051	2031	2034	2044	rBV	586415	608410	18.32%	2.255%
19	14.204	2055	2060	2066	rBV	48074	49006	1.48%	0.182%
20	14.510	2109	2112	2123	rBV	69452	88106	2.65%	0.327%
21	14.821	2160	2165	2172	rVB	90855	93686	2.82%	0.347%
22	14.898	2174	2178	2183	rVB	126651	120299	3.62%	0.446%
23	15.163	2219	2223	2227	rBV	92120	101161	3.05%	0.375%
24	15.545	2283	2288	2300	rBV2	467780	699157	21.06%	2.591%
25	15.998	2360	2365	2371	rBV2	54229	86719	2.61%	0.321%
26	16.068	2372	2377	2391	rVV8	26161	81651	2.46%	0.303%
27	16.515	2448	2453	2458	rBV2	31756	56749	1.71%	0.210%

Sum of corrected areas: 26982506

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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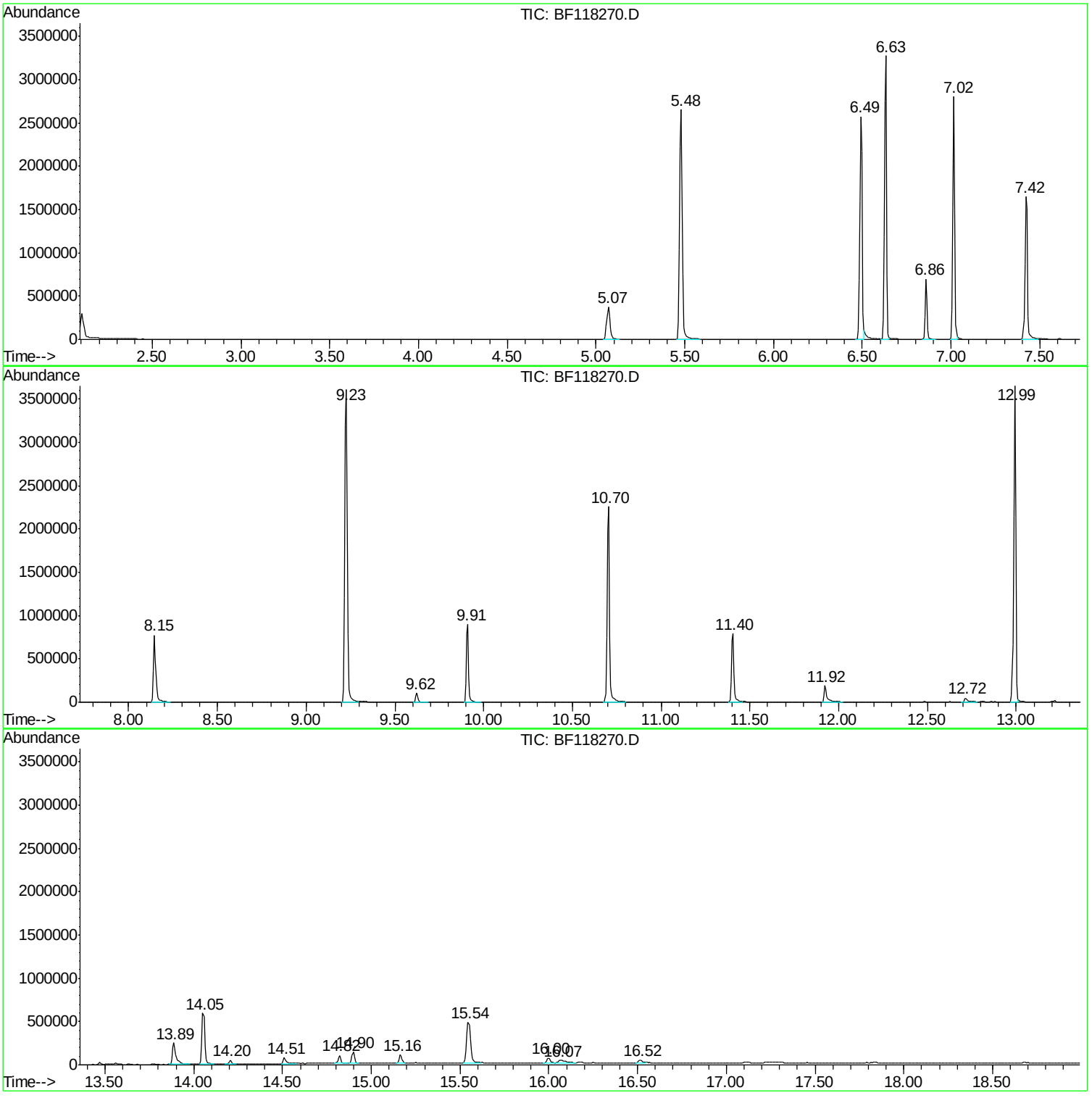
Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

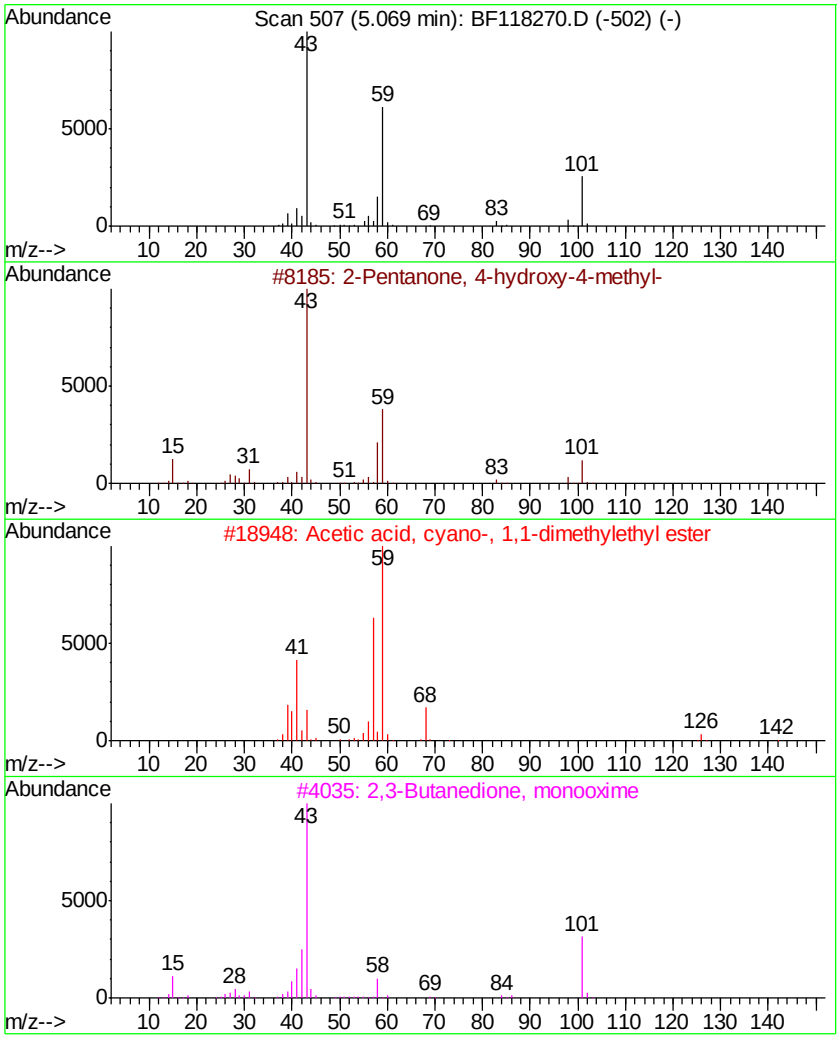
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

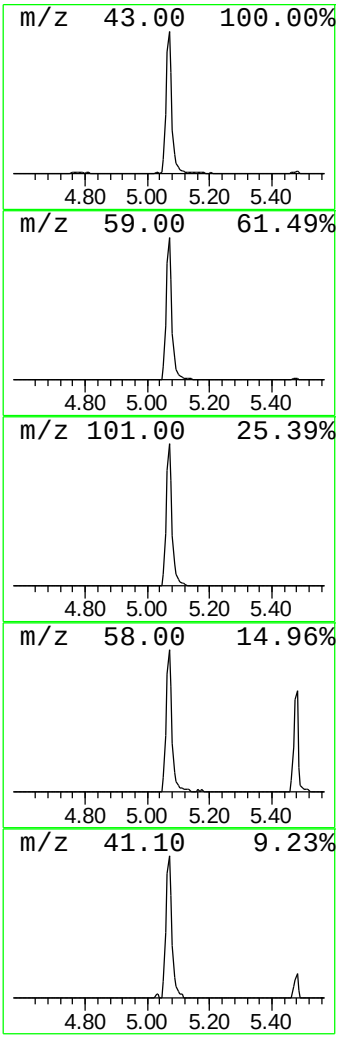
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	16.88 ng	476283	1,4-Dichlorobenzene-d4	6.86

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118270.D
Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

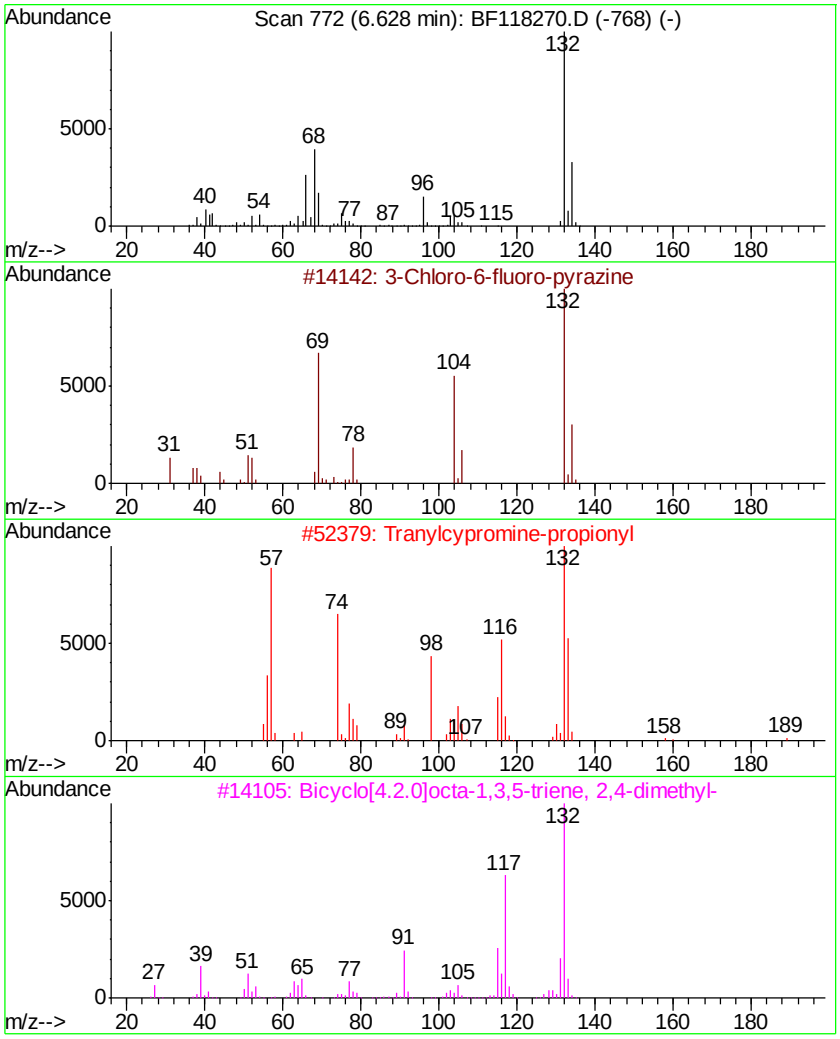
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

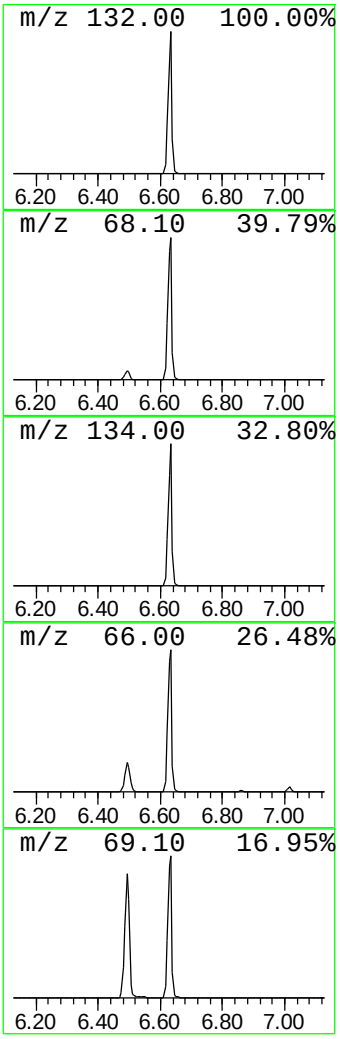
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	103.03 ng	2907680	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Xenon	132	Xe	007440-63-3	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

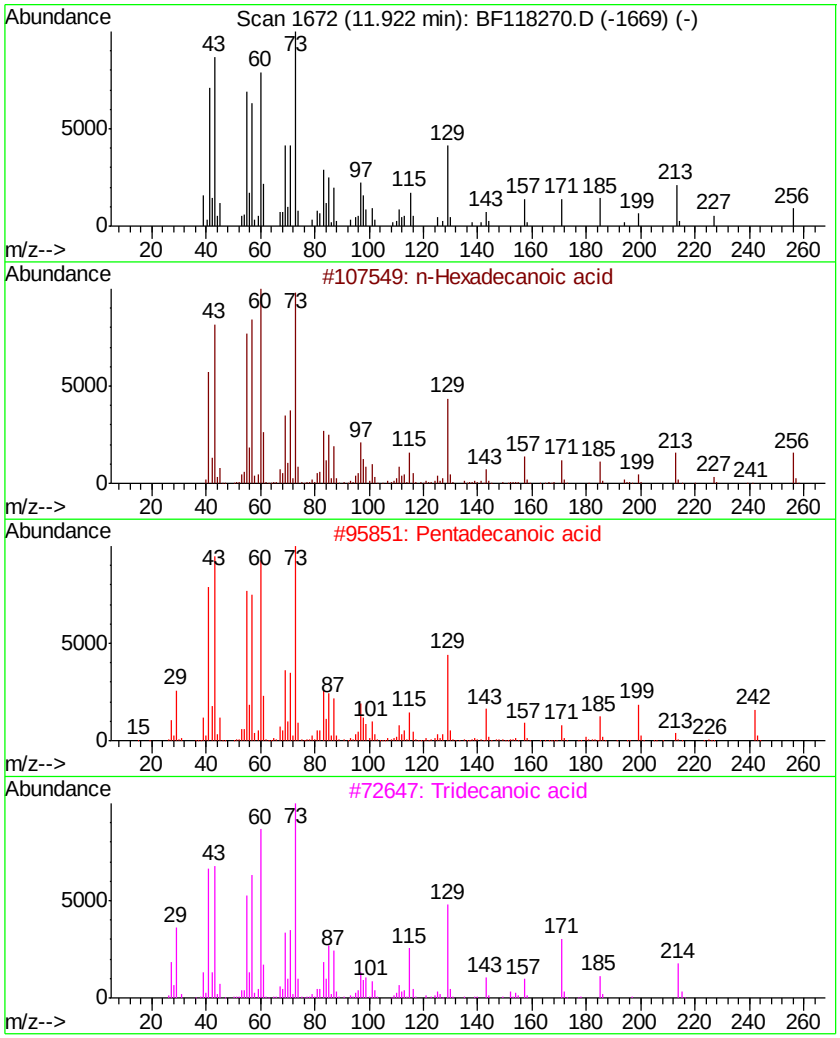
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

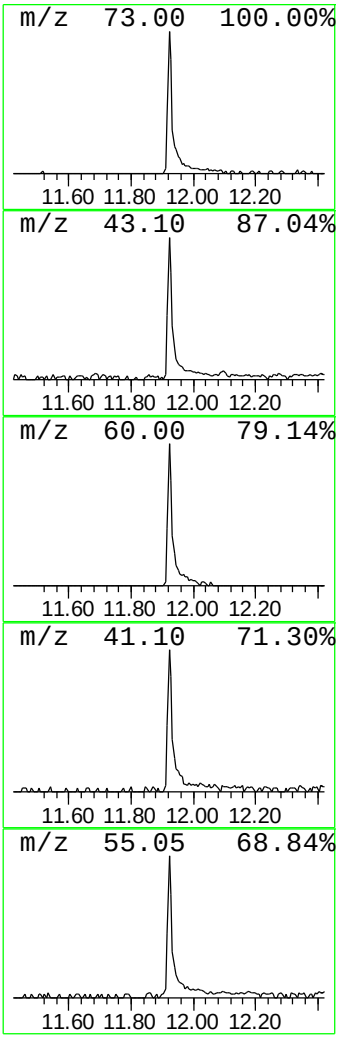
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.76 ng	234437	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

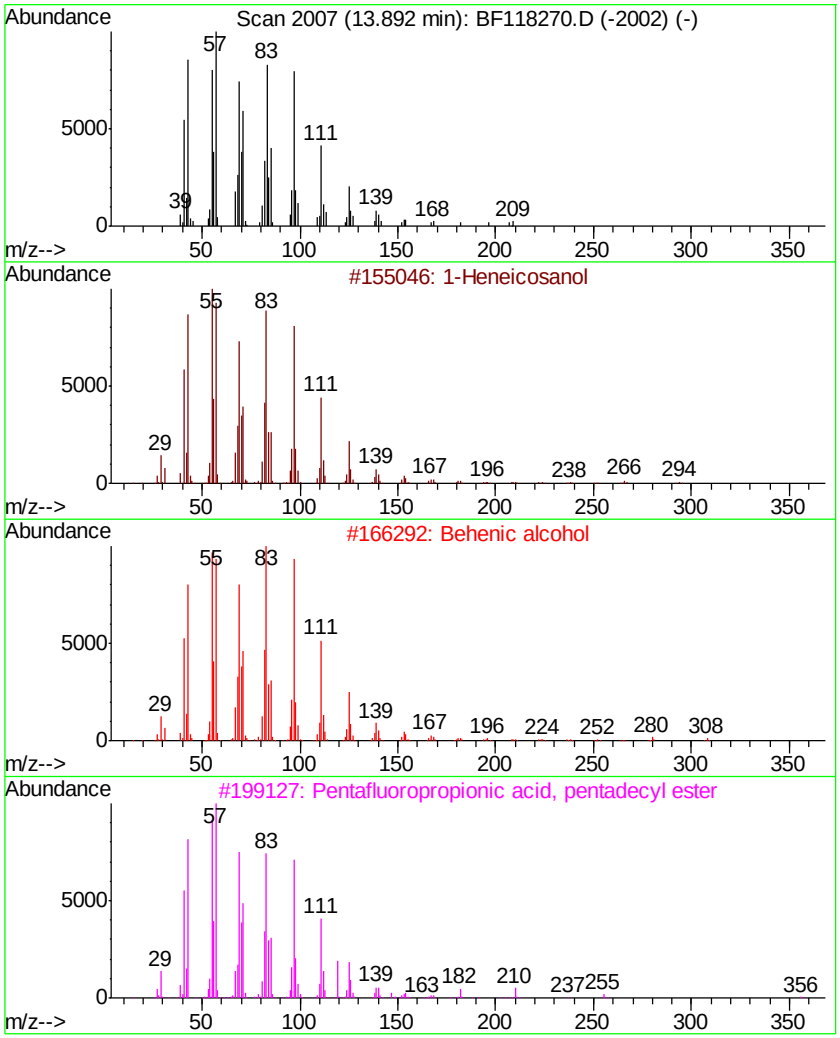
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

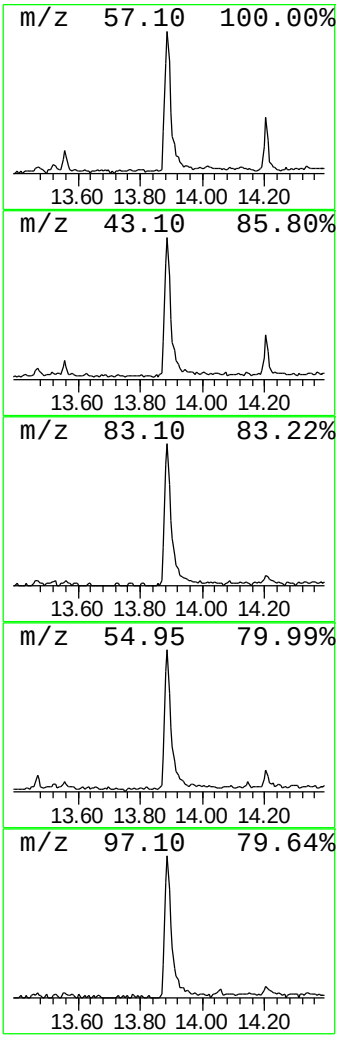
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	12.34 ng	375306	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
Data File : BF118270.D
Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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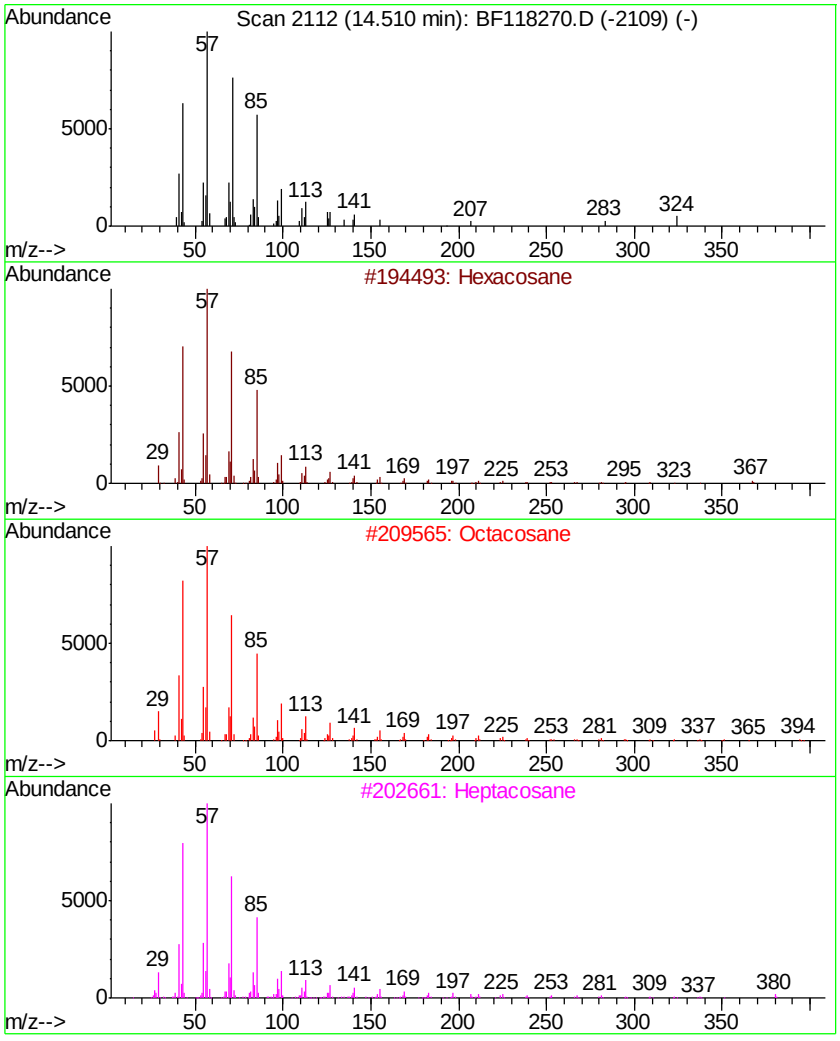
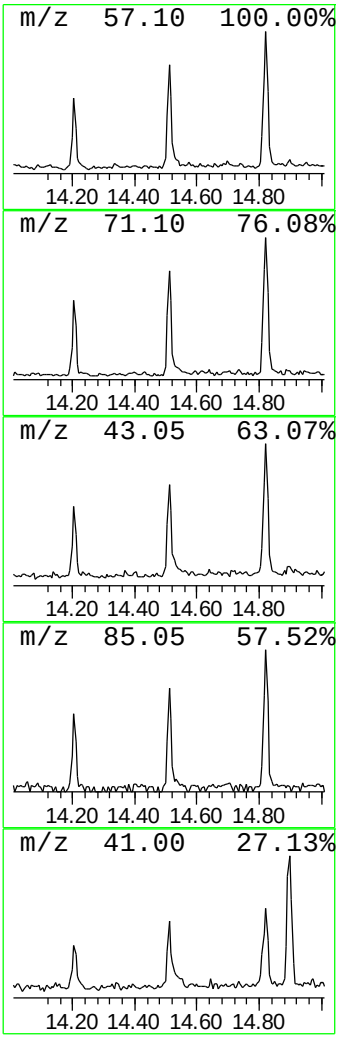
Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.90 ng	88106	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	90





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Operator : JU
Sample : K6357-02
Misc :
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Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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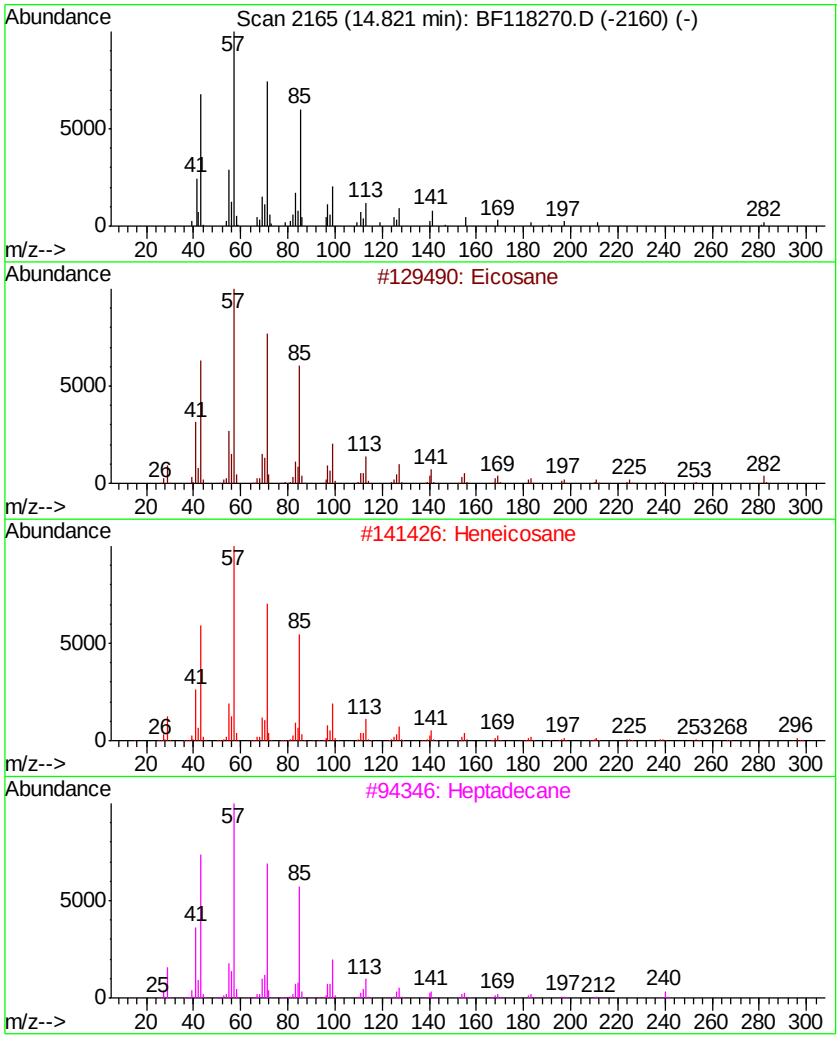
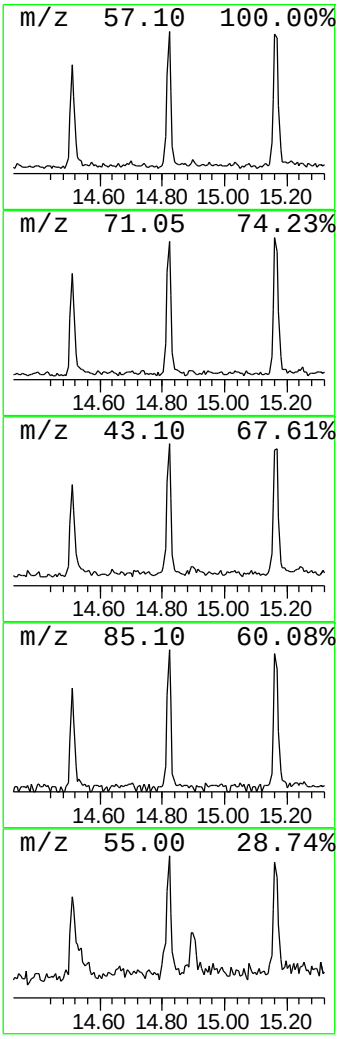
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.68 ng	93686	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





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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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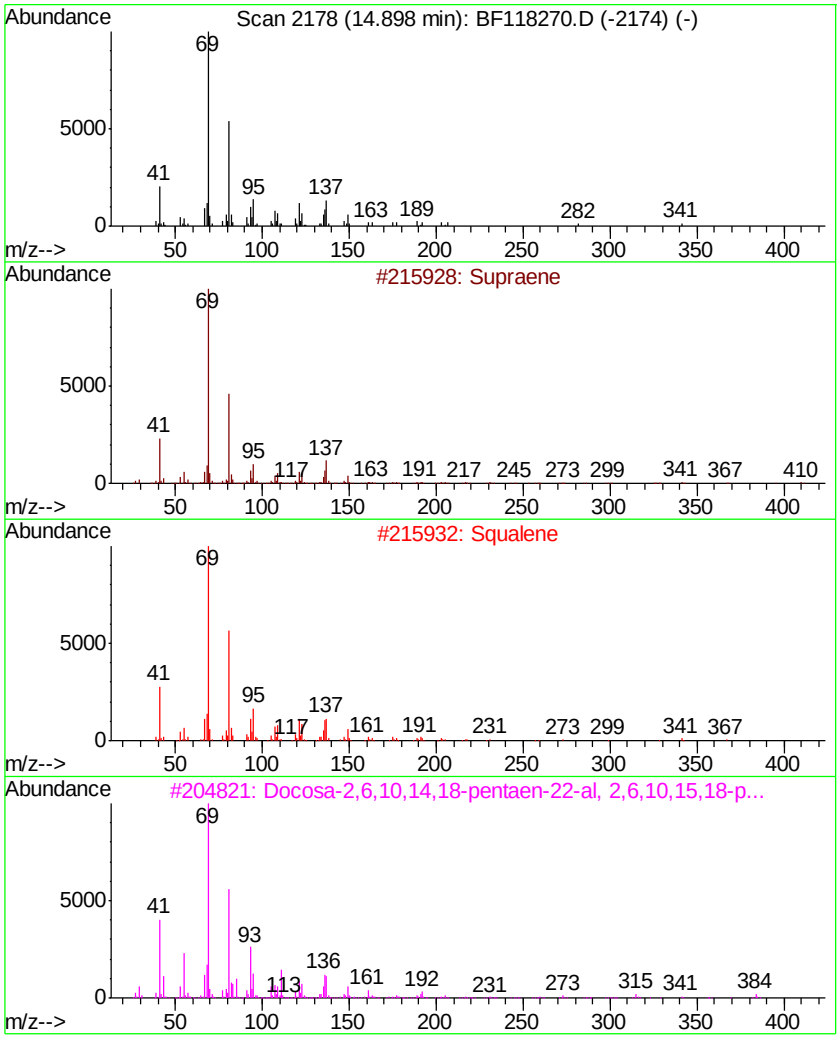
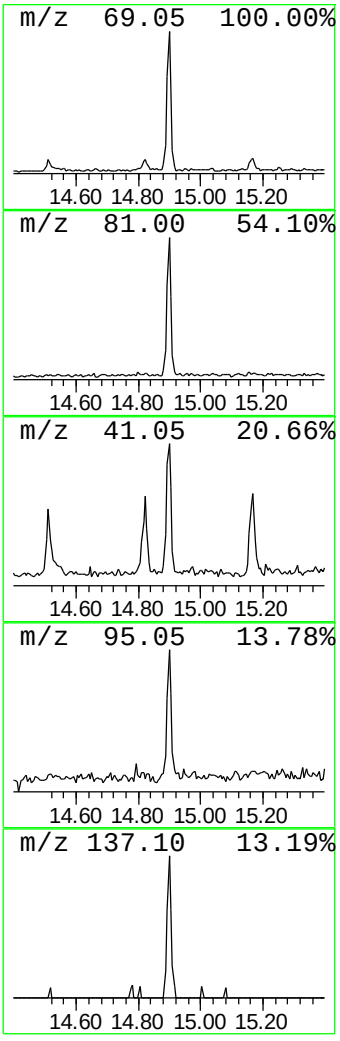
Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.44 ng	120299	Perylene-d12	15.54

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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121819\
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Misc :
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ClientSampleId : PF-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

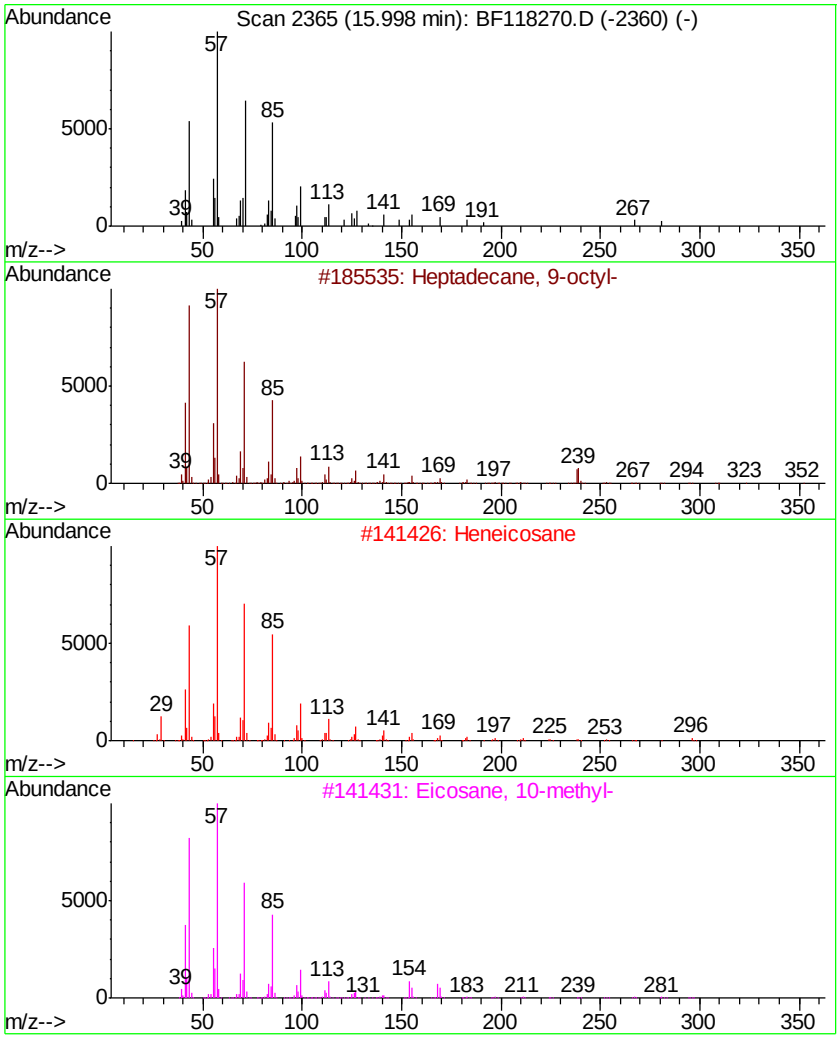
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

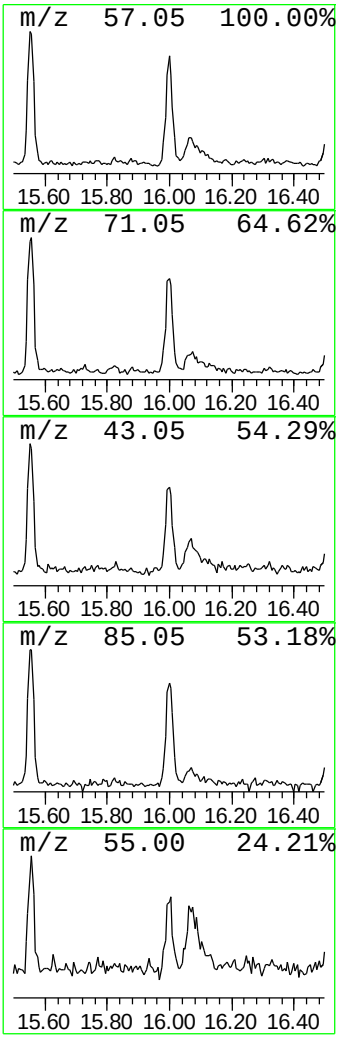
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.48 ng	86719	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Triacontane	422	C30H62	000638-68-6	90





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

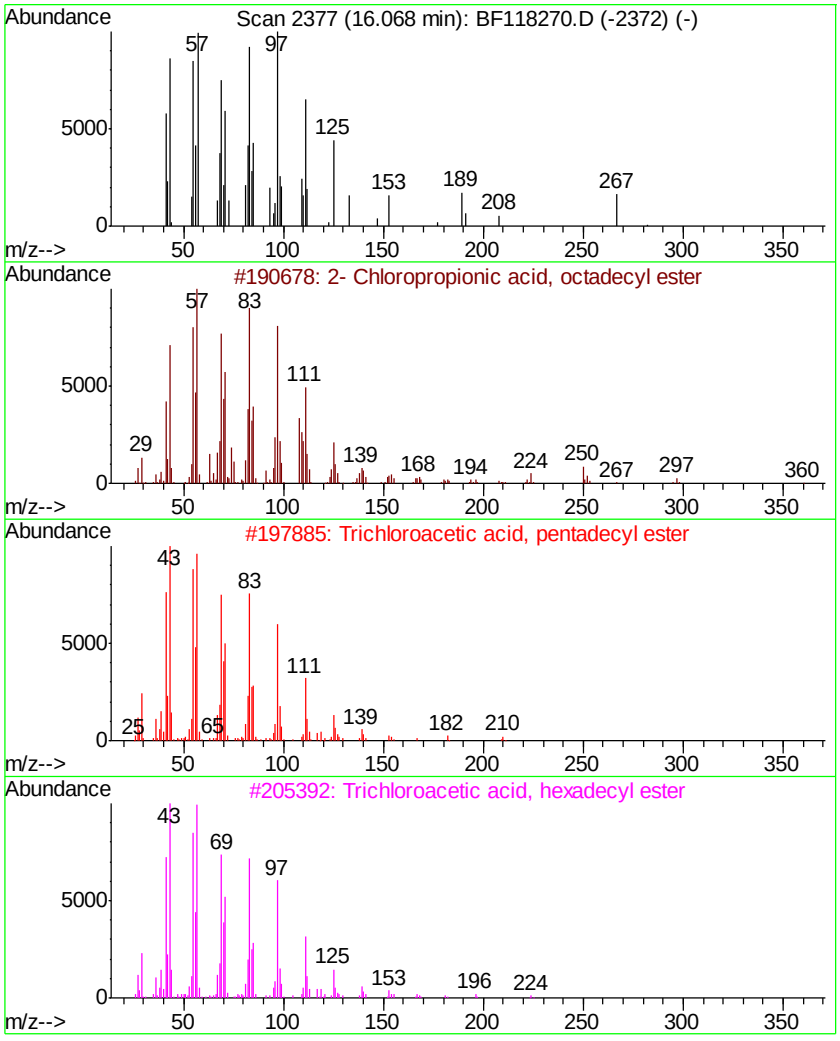
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

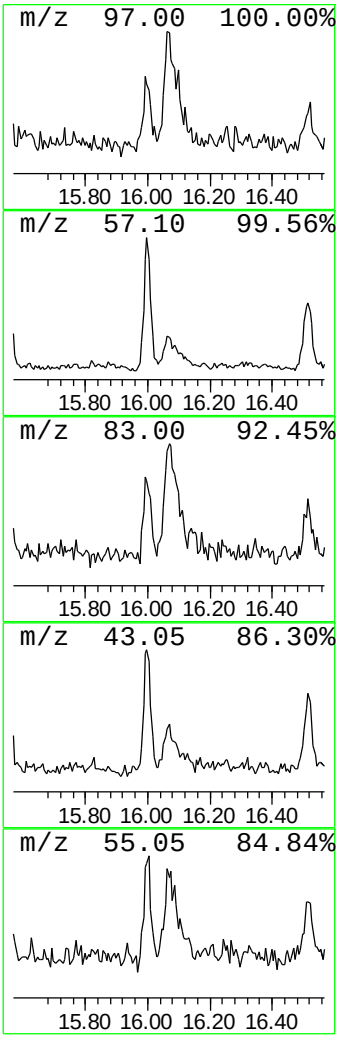
****

Peak Number 11 2- Chloropropionic acid, oc... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.34 ng	81651	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	86
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
4	1-Heptacosanol	396	C27H56O	002004-39-9	80
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121819\
Data File : BF118270.D
Acq On : 18 Dec 2019 20:30
Operator : JU
Sample : K6357-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PF-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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	16.9	ng	476283	1	6.86	564415	20.0
unknown6.63	6.63	103.0	ng	2907680	1	6.86	564415	20.0
n-Hexadecanoic acid	11.92	5.8	ng	234437	4	11.40	814399	20.0
1-Heneicosanol	13.89	12.3	ng	375306	5	14.05	608410	20.0
Hexacosane	14.51	2.9	ng	88106	5	14.05	608410	20.0
Eicosane	14.82	2.7	ng	93686	6	15.54	699157	20.0
Supraene	14.90	3.4	ng	120299	6	15.54	699157	20.0
Heptadecane, 9-oc...	16.00	2.5	ng	86719	6	15.54	699157	20.0
2- Chloropropioni...	16.07	2.3	ng	81651	6	15.54	699157	20.0