LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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	2.122	3	6	15	rVB	241805	309191	12.31%	1.398%
2	5.069	503	507	518	rVB	328686	388518	15.46%	1.757%
3	5.481	573	577	593	rBV	2177303	2054067	81.76%	9.287%
4	6.492	744	749	768	rBV	2341494	2184952	86.97%	9.879%
5	6.628	768	772	776	rBV	2461870	2337237	93.03%	10.567%
6	6.857	808	811	819	rBV	695069	598329	23.82%	2.705%
7	7.016	834	838	841	rBV	2284092	1836088	73.08%	8.301%
8	7.422	903	907	920	rBV	1441009	1332753	53.05%	6.026%
9	8.145	1026	1030	1053	rBV	829787	767907	30.57%	3.472%
10	9.222	1209	1213	1225	rBV	2750176	2512277	100.00%	11.359%
11	9.622	1277	1281	1289	rBV	96820	97520	3.88%	0.441%
12	9.910	1326	1330	1344	rVB	892859	817462	32.54%	3.696%
13	10.698	1461	1464	1480	rBV	1424458	1421433	56.58%	6.427%
14	11.404	1580	1584	1593	rBV	755431	741585	29.52%	3.353%
15	11.922	1669	1672	1684	rBV	121902	151159	6.02%	0.683%
16	12.716	1804	1807	1814	rBV6	21219	35539	1.41%	0.161%
17	12.992	1850	1854	1857	rBV	2673316	2196816	87.44%	9.932%
18	13.886	2003	2006	2014	rBV	224397	312491	12.44%	1.413%
19	14.057	2031	2035	2044	rBV	779646	737281	29.35%	3.333%
20	14.210	2058	2061	2065	rBV	48281	57021	2.27%	0.258%
21	14.515	2110	2113	2116	rBV	67177	68657	2.73%	0.310%
22	14.821	2160	2165	2168	rBV2	81795	102059	4.06%	0.461%
23	14.904	2176	2179	2182	rVB	54751	49801	1.98%	0.225%
24	15.168	2221	2224	2227	rVB	75715	82444	3.28%	0.373%
25	15.545	2283	2288	2298	rBV	522704	822628	32.74%	3.719%
26	16.004	2362	2366	2372	rVB	68981	102685	4.09%	0.464%

Sum of corrected areas: 22117900

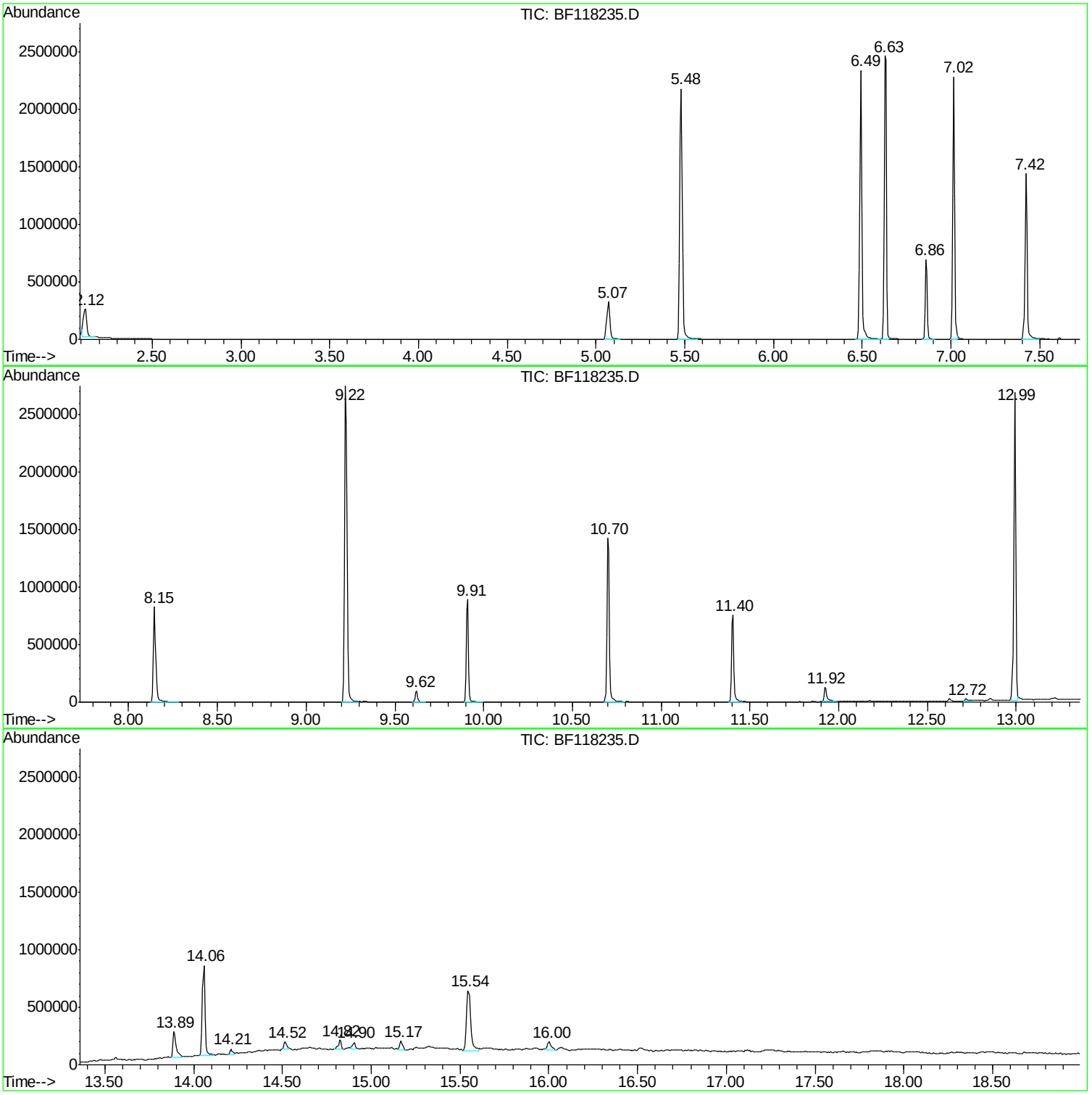
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

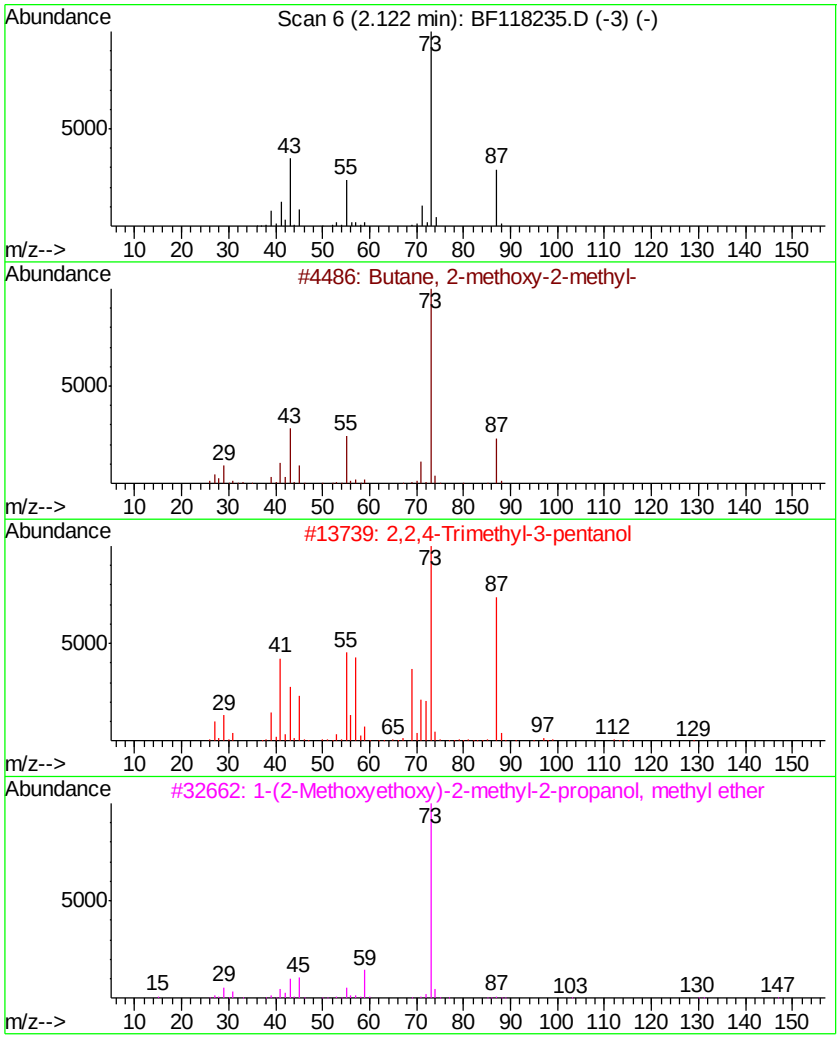
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

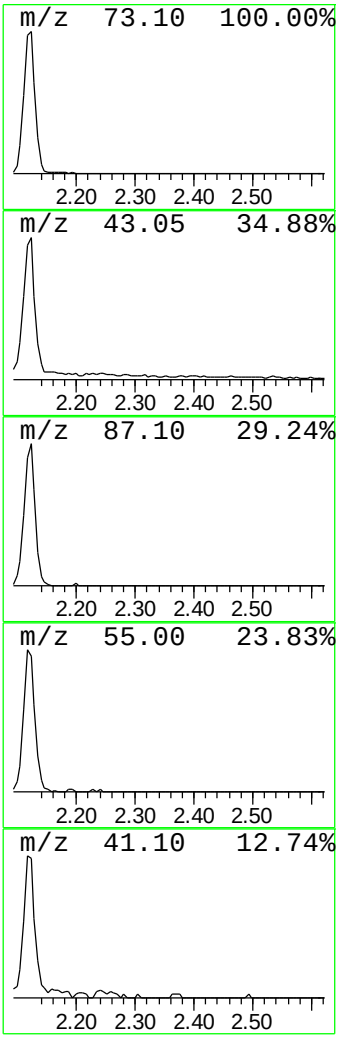
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	10.34 ng	309191	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17





Library Search Compound Report

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Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

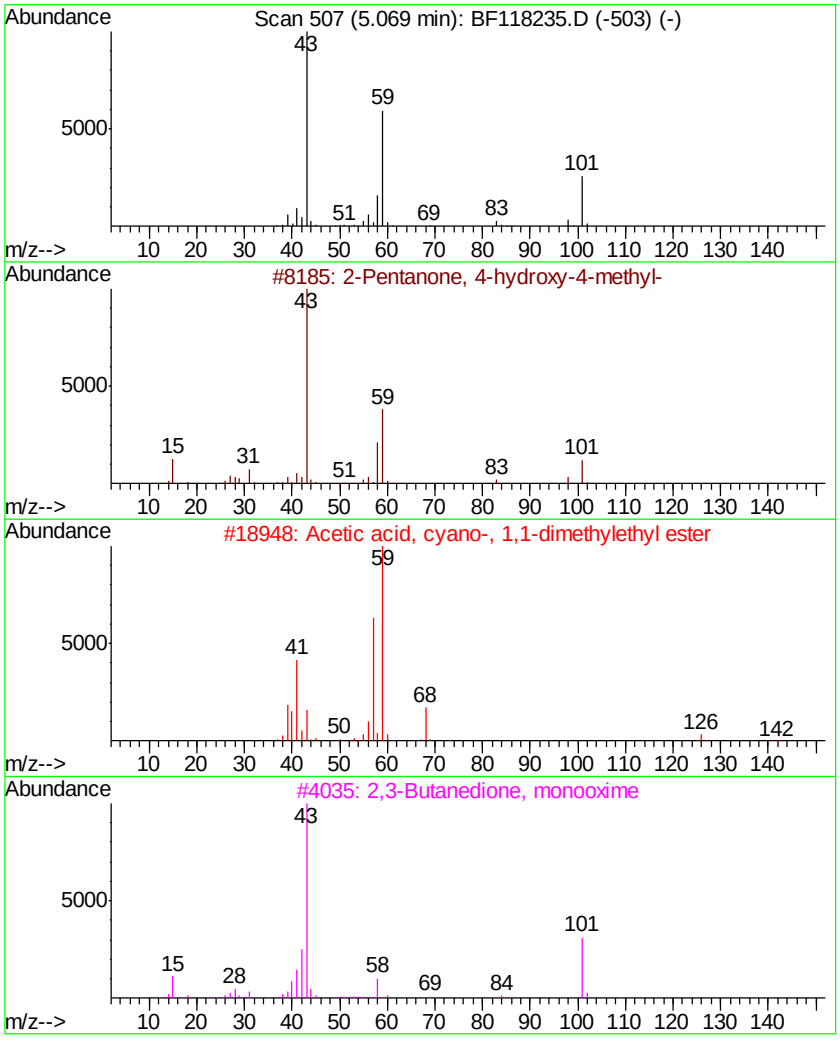
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

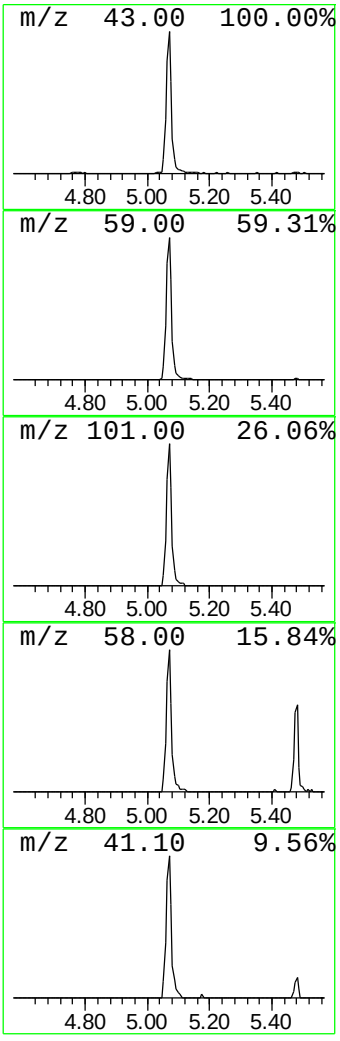
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.99 ng	388518	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

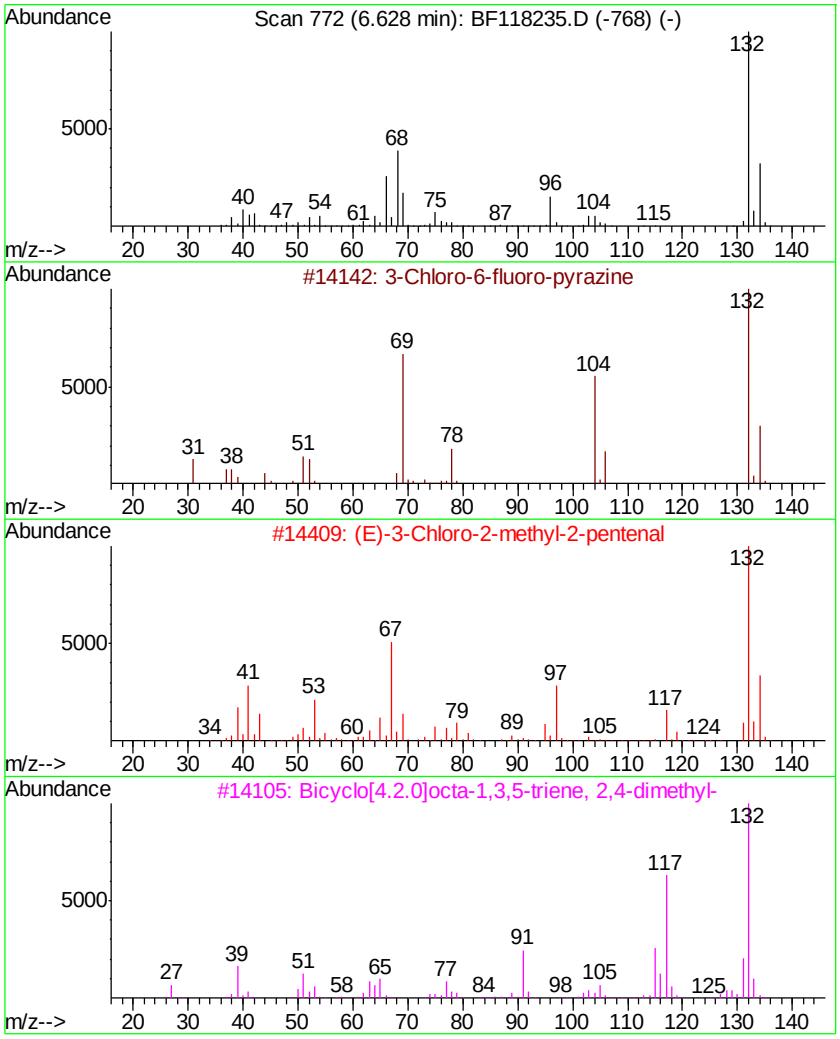
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

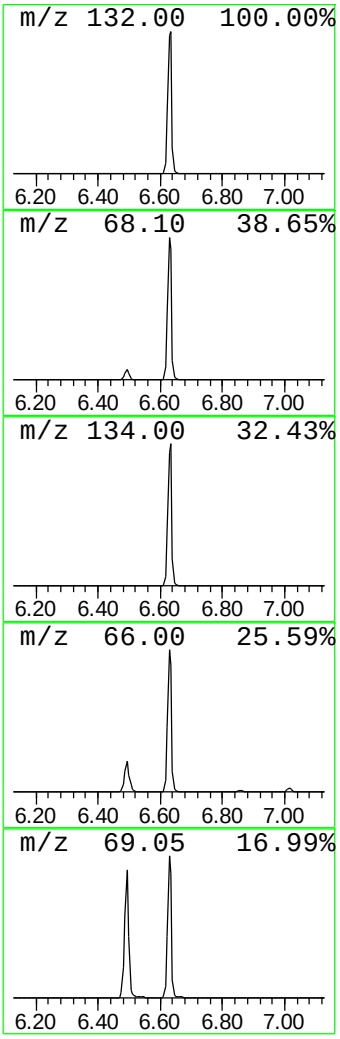
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.13 ng	2337240	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
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Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

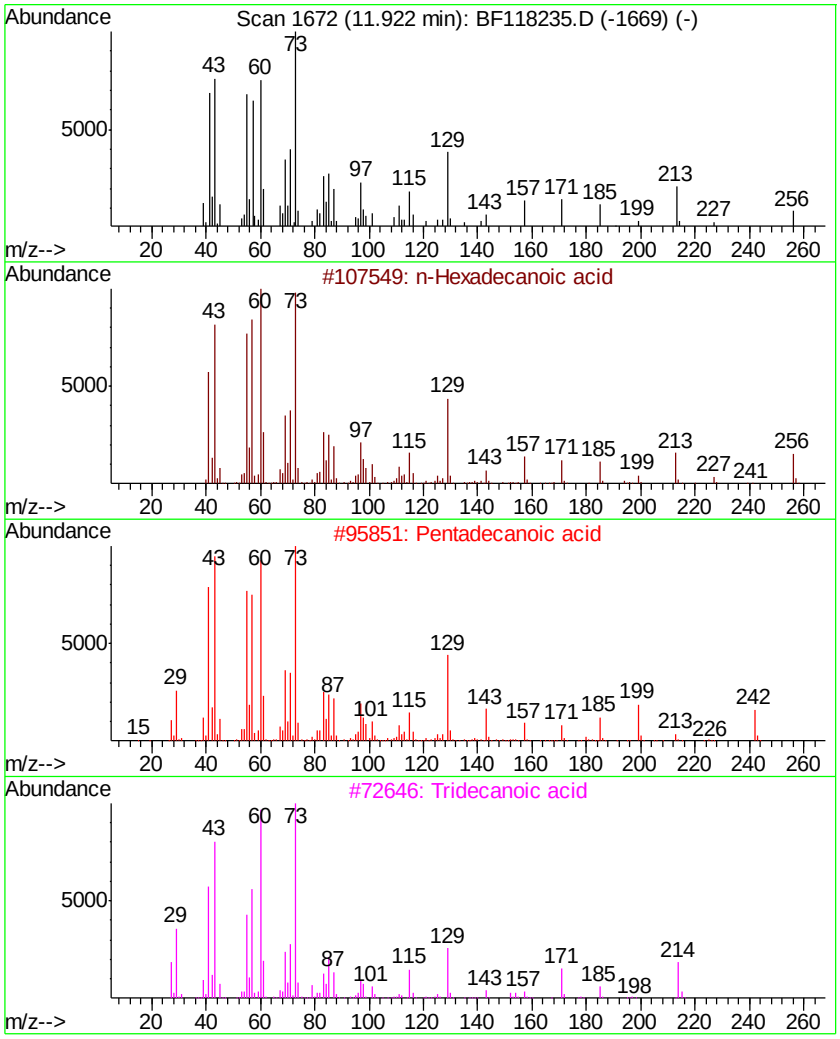
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

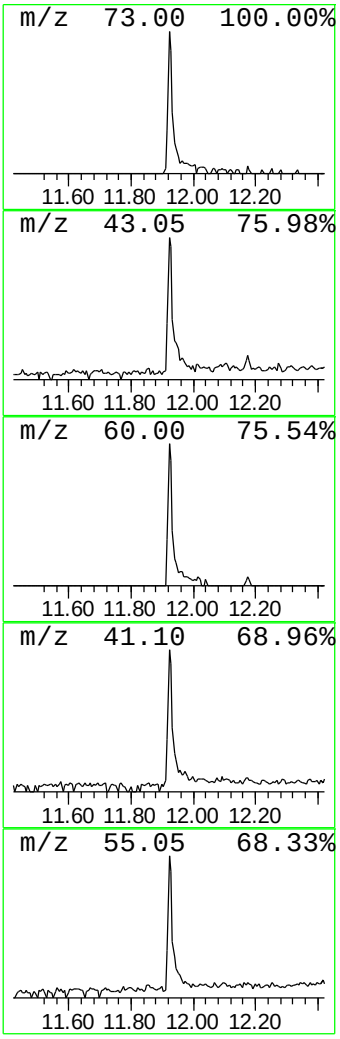
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.08 ng	151159	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
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Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

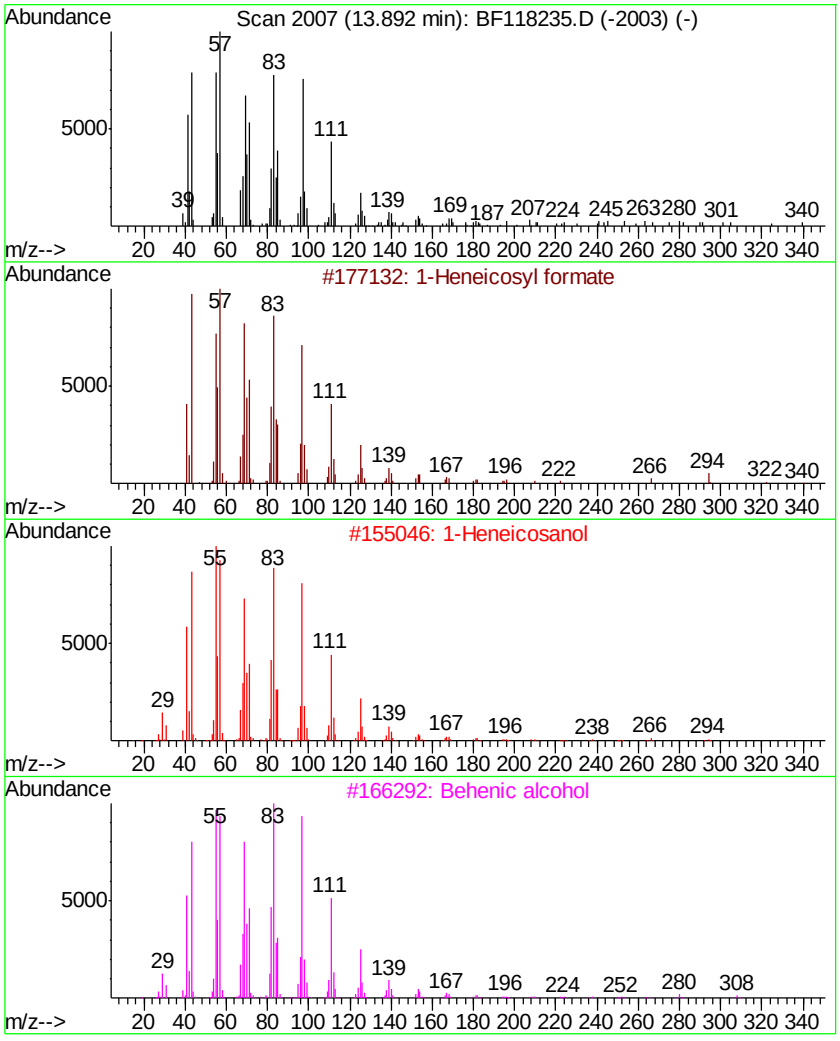
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

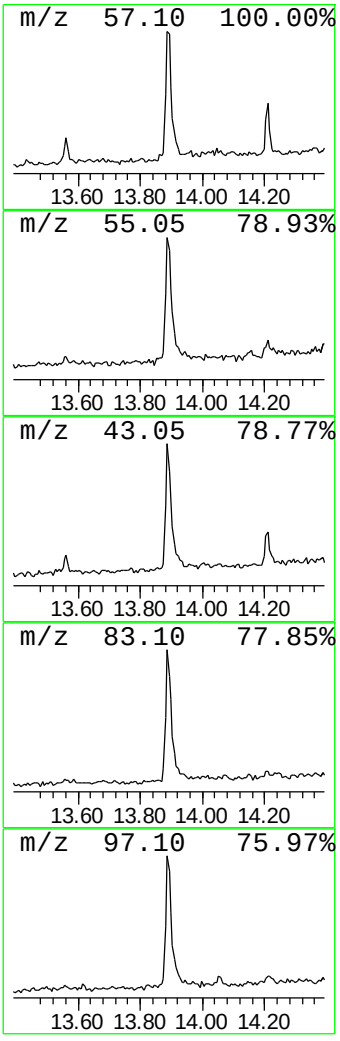
****

Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	8.48 ng	312491	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Library Search Compound Report

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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

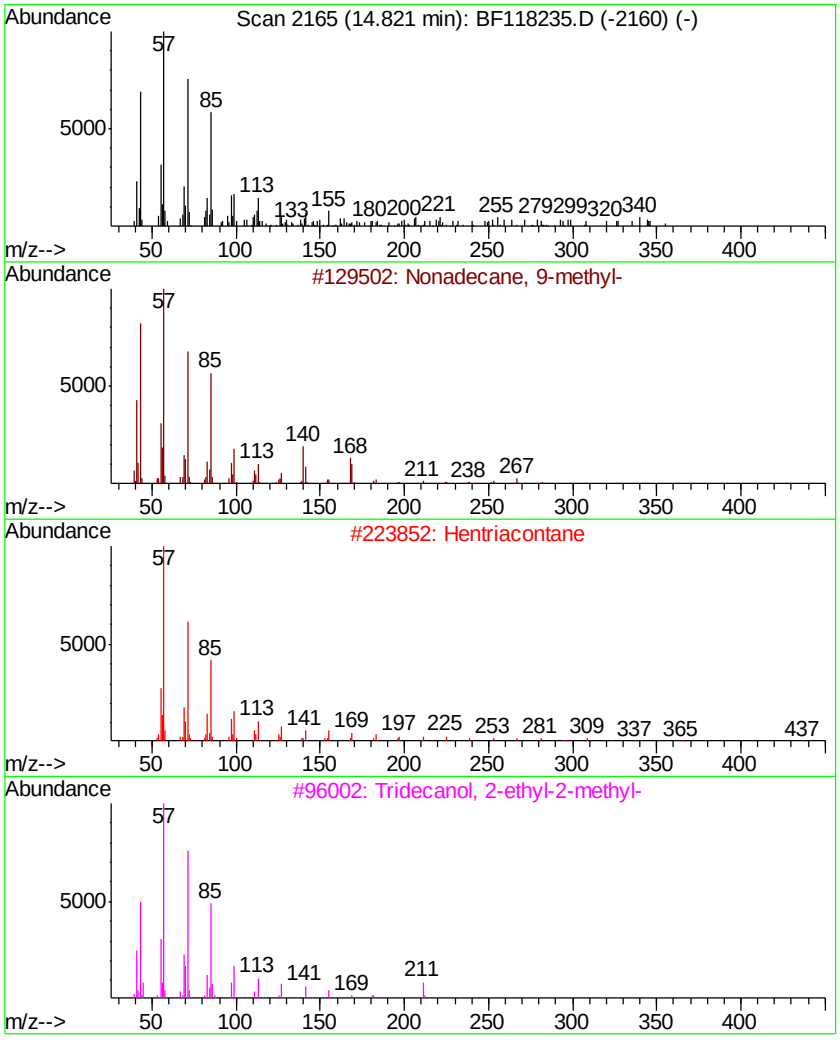
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

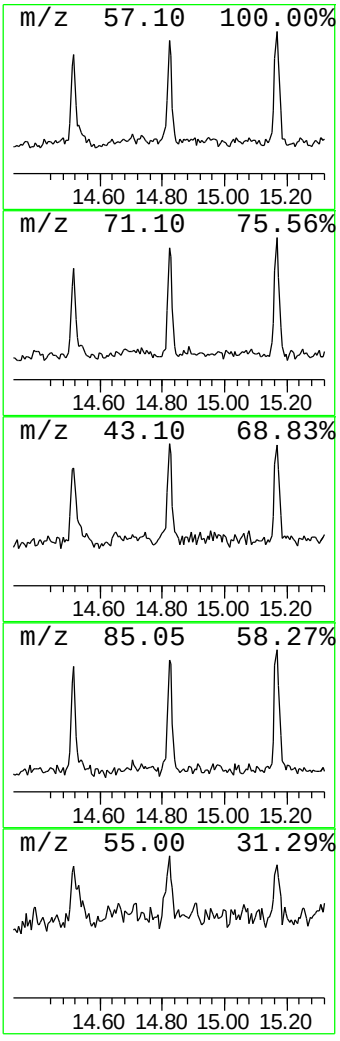
****

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.48 ng	102059	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Eicosane	282	C20H42	000112-95-8	87





Library Search Compound Report

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Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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

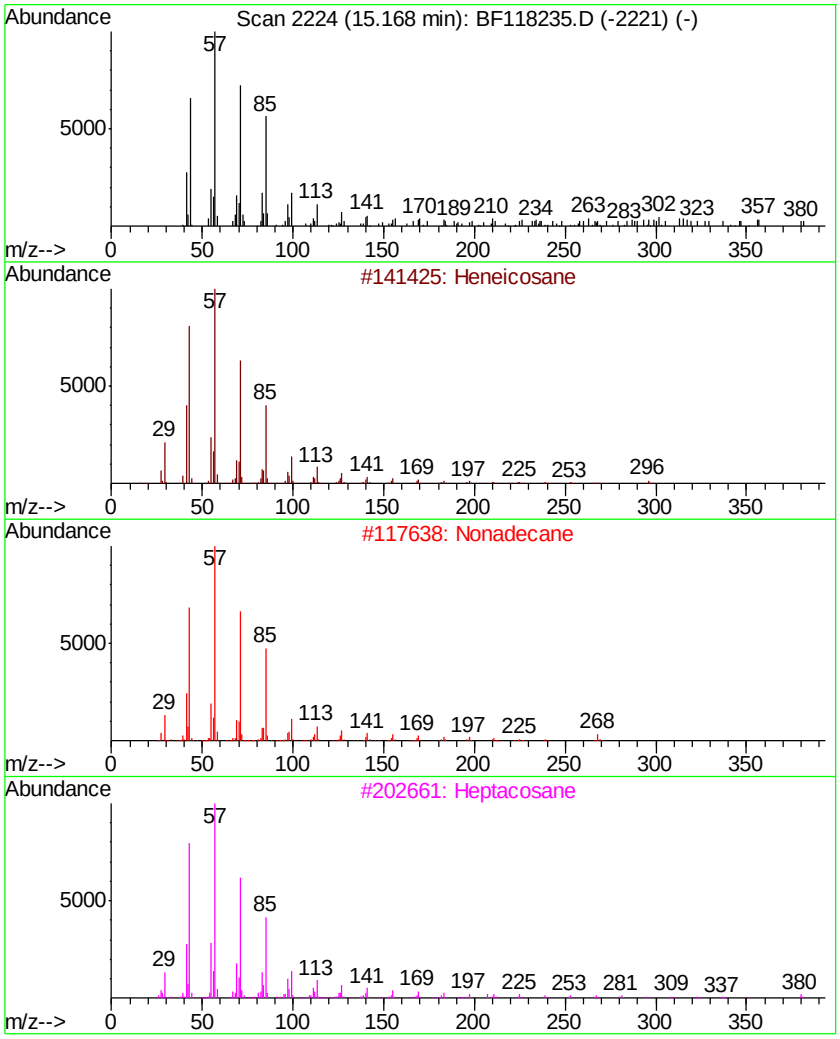
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

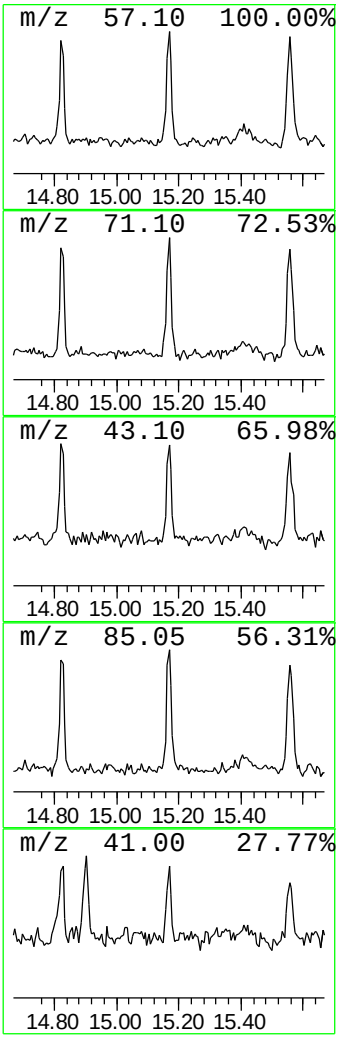
****

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.00 ng	82444	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Nonadecane	268	C19H40	000629-92-5	96
3	Heptacosane	380	C27H56	000593-49-7	95
4	Hexadecane	226	C16H34	000544-76-3	91
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83





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Sample : K6333-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

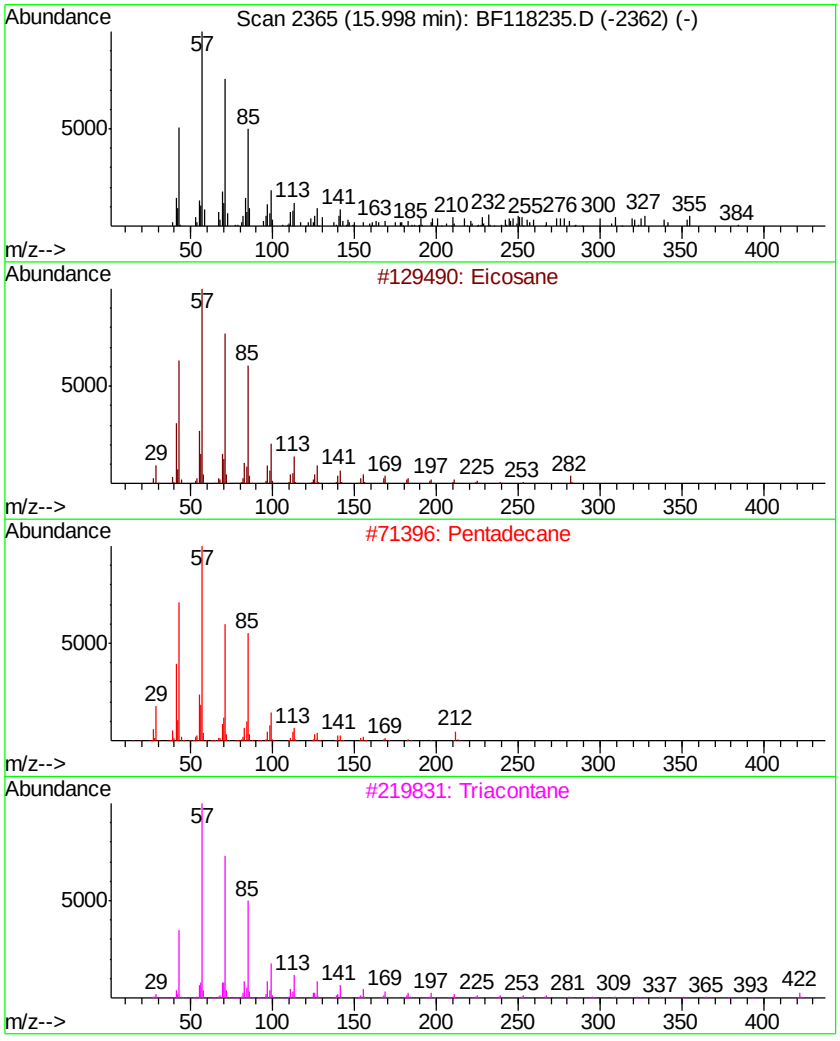
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

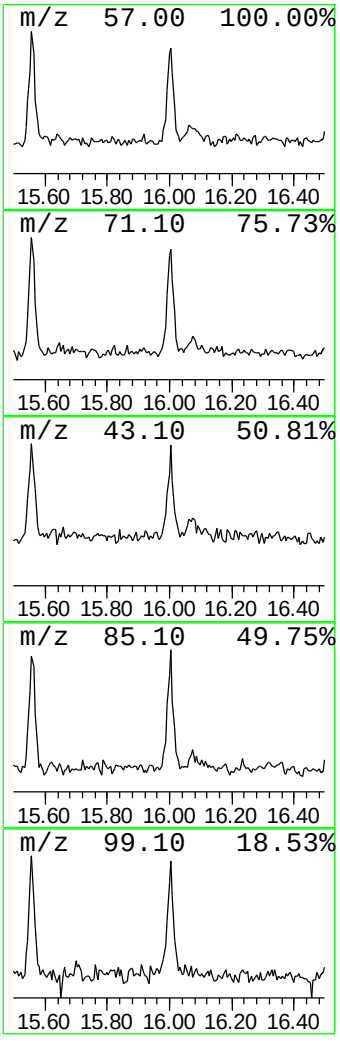
****

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.50 ng	102685	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Pentadecane	212	C15H32	000629-62-9	81
3	Triacontane	422	C30H62	000638-68-6	74
4	Heneicosane, 10-methyl-	310	C22H46	013287-25-7	74
5	Heneicosane	296	C21H44	000629-94-7	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
Data File : BF118235.D
Acq On : 17 Dec 2019 19:23
Operator : JU
Sample : K6333-04
Misc :
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Instrument : BNA_F
ClientSampleId : TP-1A-COMP

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
Butane, 2-methoxy...	2.12	10.3	ng	309191	1	6.86	598329	20.0
2-Pentanone, 4-hy...	5.07	13.0	ng	388518	1	6.86	598329	20.0
unknown6.63	6.63	78.1	ng	2337240	1	6.86	598329	20.0
n-Hexadecanoic acid	11.92	4.1	ng	151159	4	11.40	741585	20.0
1-Heneicosyl formate	13.89	8.5	ng	312491	5	14.06	737281	20.0
Nonadecane, 9-met...	14.82	2.5	ng	102059	6	15.54	822628	20.0
Heneicosane	15.17	2.0	ng	82444	6	15.54	822628	20.0
Eicosane	16.00	2.5	ng	102685	6	15.54	822628	20.0