LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

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-BF082720.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	2.158	7	12	29	rVB	1866338	2443184	34.70%	4.476%
2	5.081	505	509	517	rVB	95393	118228	1.68%	0.217%
3	5.475	571	576	579	rBV	5385938	5014252	71.22%	9.185%
4	6.481	741	747	750	rBV	5218732	5222686	74.18%	9.567%
5	6.681	778	781	787	rBV	158023	127843	1.82%	0.234%
6	6.857	808	811	817	rVB	2289457	1809556	25.70%	3.315%
7	7.422	901	907	910	rBV	3862663	3579821	50.85%	6.558%
8	8.140	1025	1029	1033	rBV	2765734	2384653	33.87%	4.368%
9	9.222	1207	1213	1216	rBV	6971631	6669271	94.73%	12.217%
10	9.610	1275	1279	1282	rBV	568580	441240	6.27%	0.808%
11	9.898	1323	1328	1331	rBV	3240007	2746680	39.01%	5.032%
12	10.681	1456	1461	1465	rBV	4568167	4053943	57.58%	7.426%
13	10.816	1479	1484	1491	rVB	71406	98716	1.40%	0.181%
14	11.380	1576	1580	1583	rBV	3404802	2865440	40.70%	5.249%
15	11.910	1667	1670	1674	rBV	529181	541905	7.70%	0.993%
16	12.086	1697	1700	1703	rBV	92857	74437	1.06%	0.136%
17	12.475	1763	1766	1770	rVB	89396	74110	1.05%	0.136%
18	12.592	1782	1786	1788	rBV	76451	76820	1.09%	0.141%
19	12.698	1800	1804	1811	rBV2	115085	174842	2.48%	0.320%
20	12.974	1846	1851	1854	rBV	6686459	7040296	100.00%	12.897%
21	13.545	1943	1948	1952	rBV3	69715	89527	1.27%	0.164%
22	13.869	1999	2003	2014	rBV	1629170	1729647	24.57%	3.169%
23	14.021	2024	2029	2032	rBV	2445303	2412005	34.26%	4.418%
24	14.192	2055	2058	2062	rBV2	129667	143384	2.04%	0.263%
25	14.504	2107	2111	2117	rBV	233245	293047	4.16%	0.537%
26	14.786	2155	2159	2161	rBV	244532	285054	4.05%	0.522%
27	14.886	2173	2176	2179	rVB	93453	101666	1.44%	0.186%
28	14.951	2184	2187	2192	rVB	218889	231091	3.28%	0.423%
29	15.151	2217	2221	2222	rBV	194087	192891	2.74%	0.353%
30	15.174	2222	2225	2232	rVB	321375	440932	6.26%	0.808%
31	15.486	2273	2278	2283	rBV	1641196	1910870	27.14%	3.500%
32	15.533	2283	2286	2291	rVB	83509	99710	1.42%	0.183%
33	15.739	2317	2321	2326	rVB	139954	182810	2.60%	0.335%
34	15.974	2357	2361	2365	rBV	148662	205189	2.91%	0.376%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

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-BF082720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.021	2365	2369	2378	rVB	228538	404485	5.75%	0.741%
36	16.774	2493	2497	2505	rVB2	67325	132144	1.88%	0.242%
37	17.551	2624	2629	2640	rBV9	74436	176447	2.51%	0.323%

Sum of corrected areas: 54588822

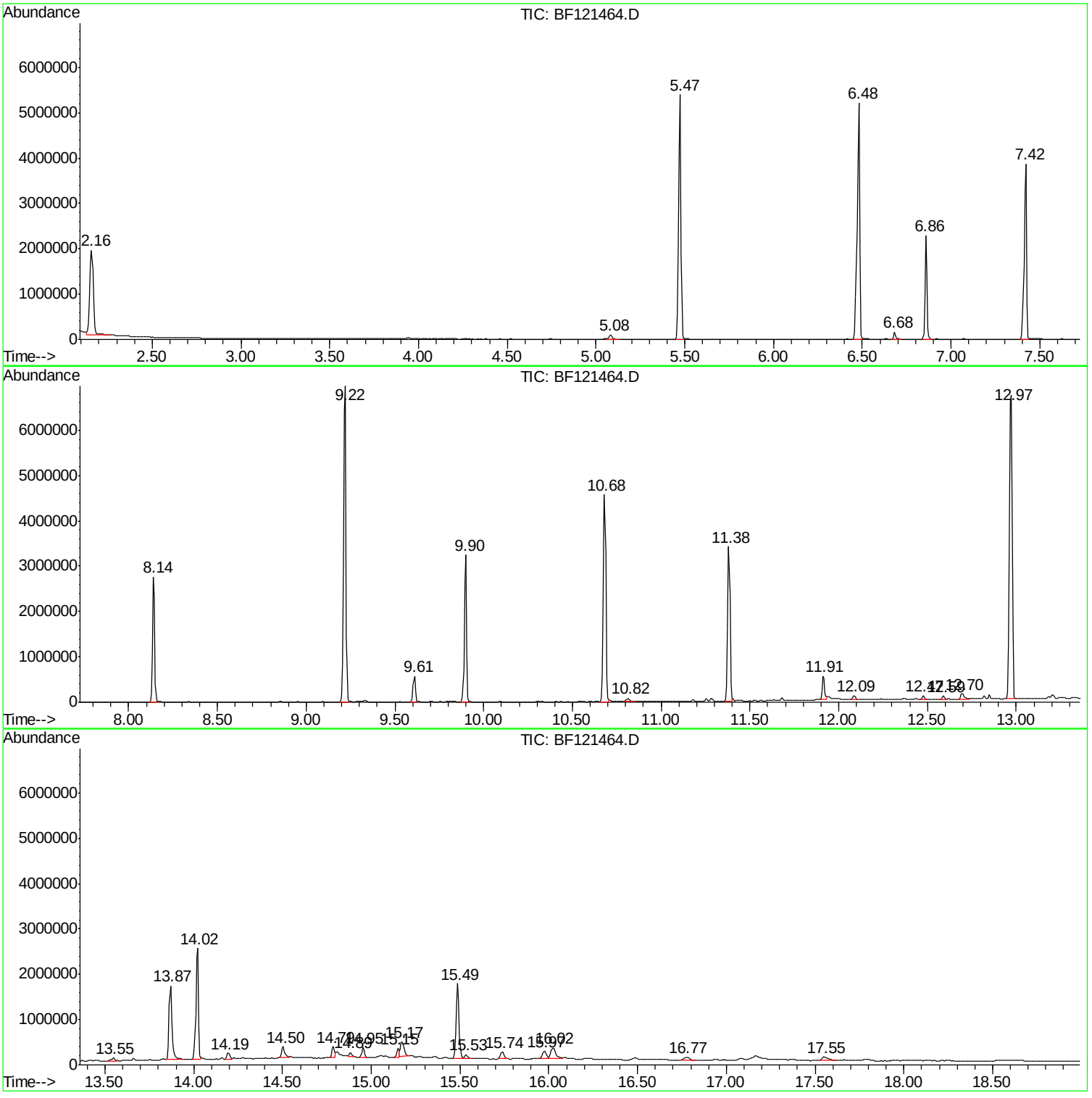
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.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\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
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Misc :
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Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

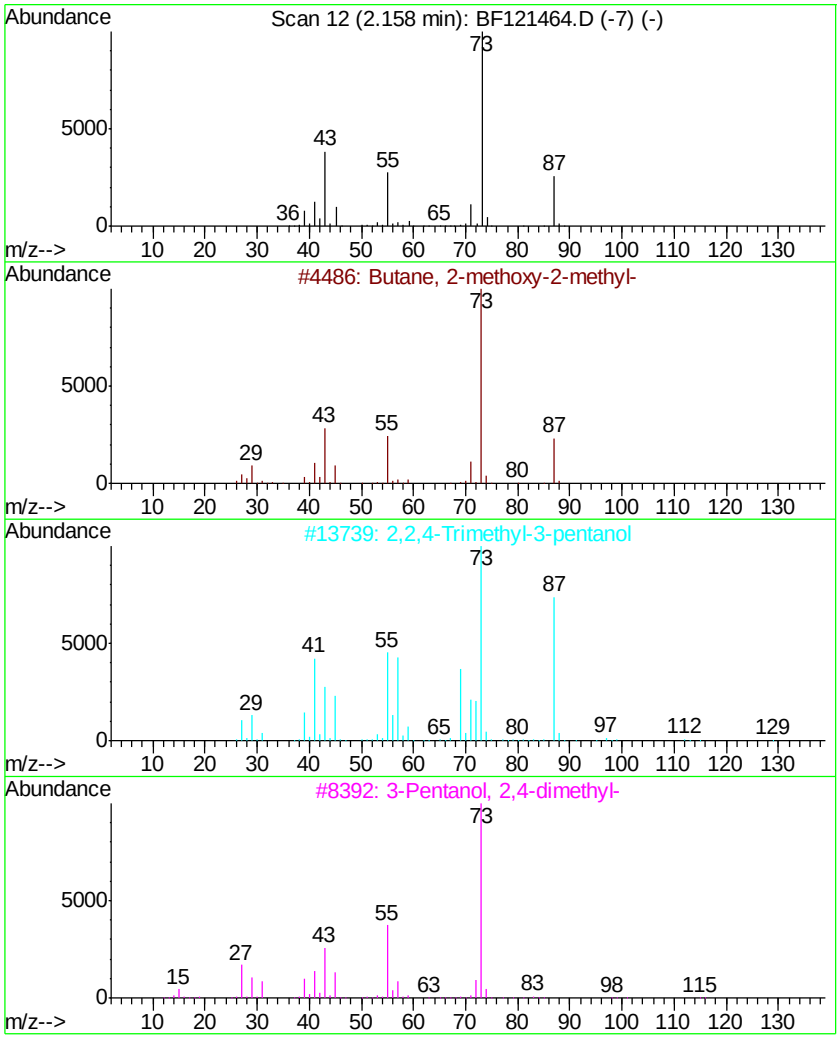
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

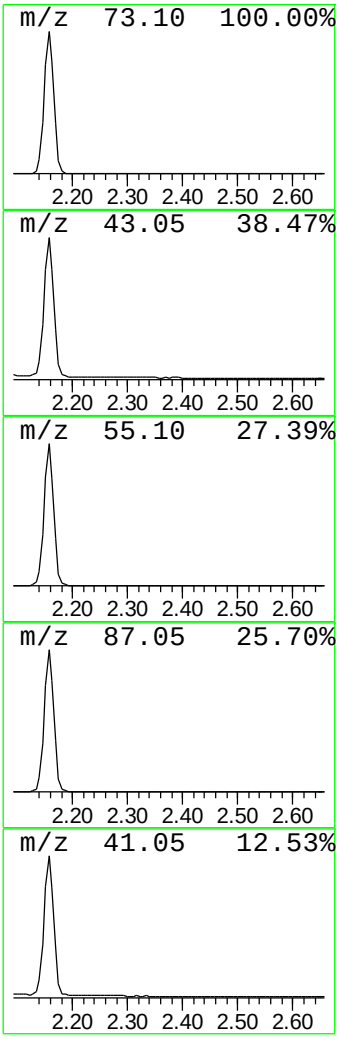
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	27.00 ng	2443180	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.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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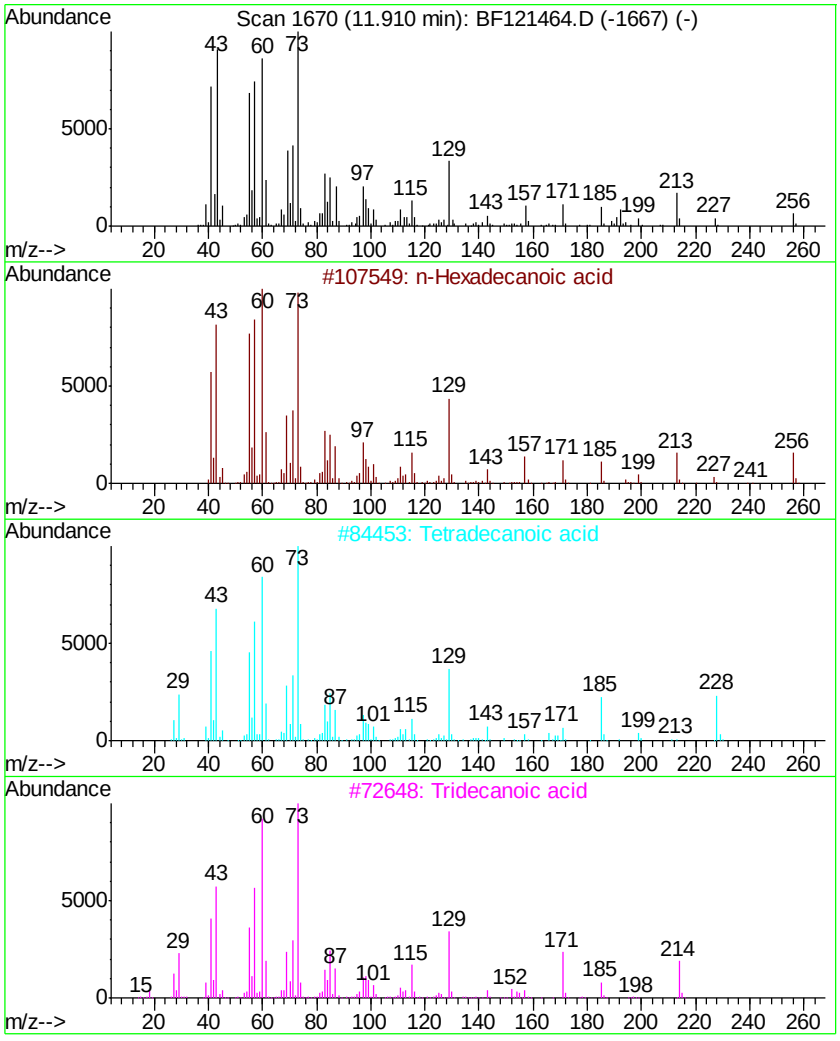
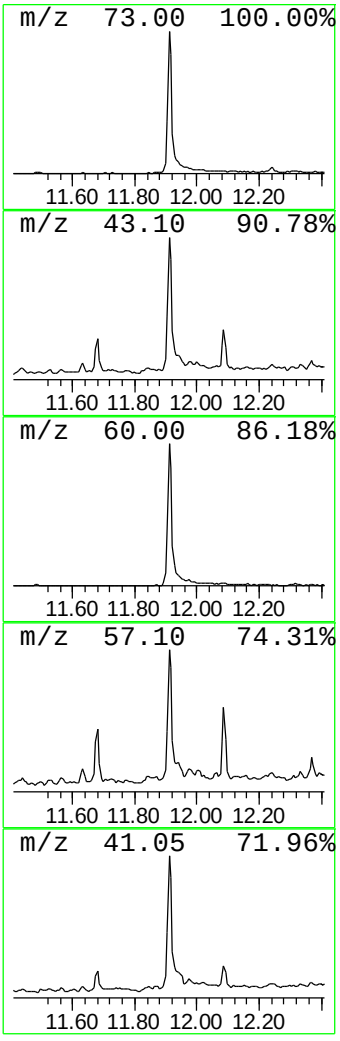
Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	3.78 ng	541905	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
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Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

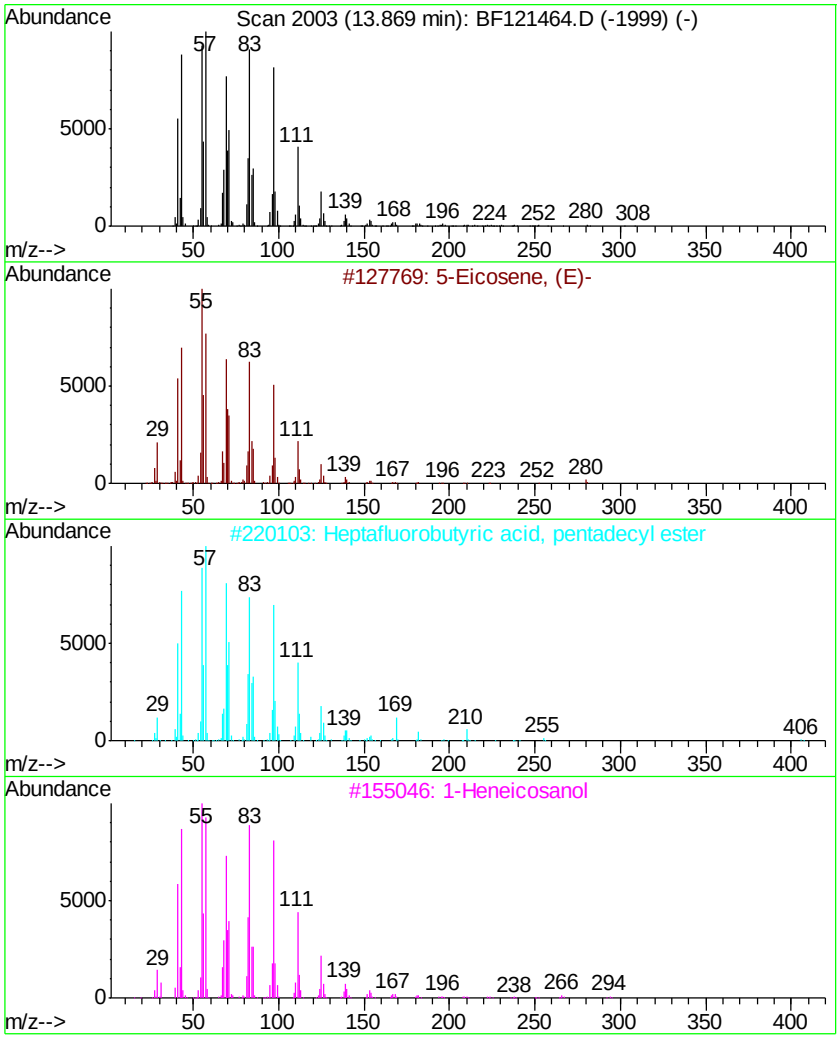
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

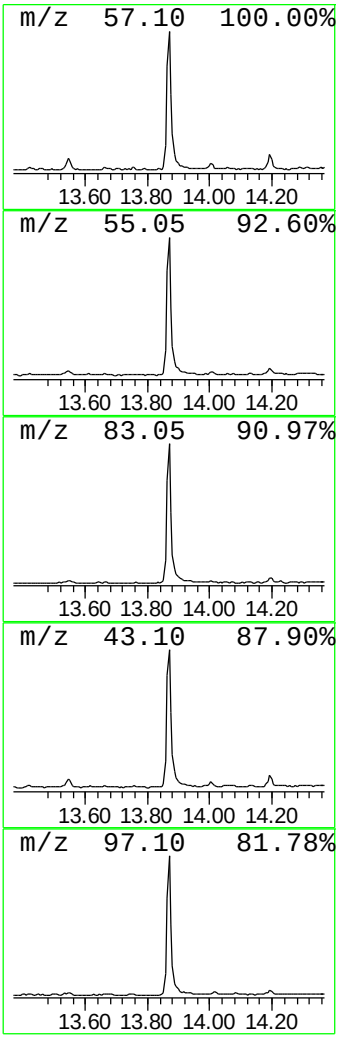
****

Peak Number 3 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	14.34 ng	1729650	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

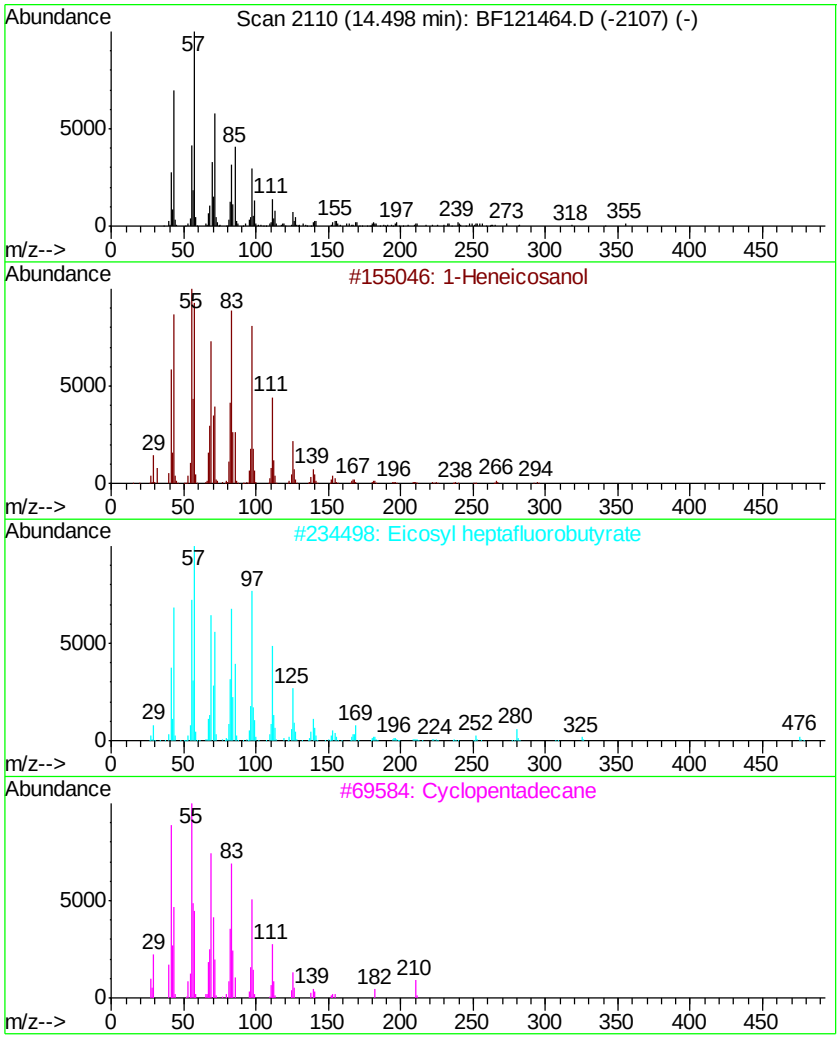
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

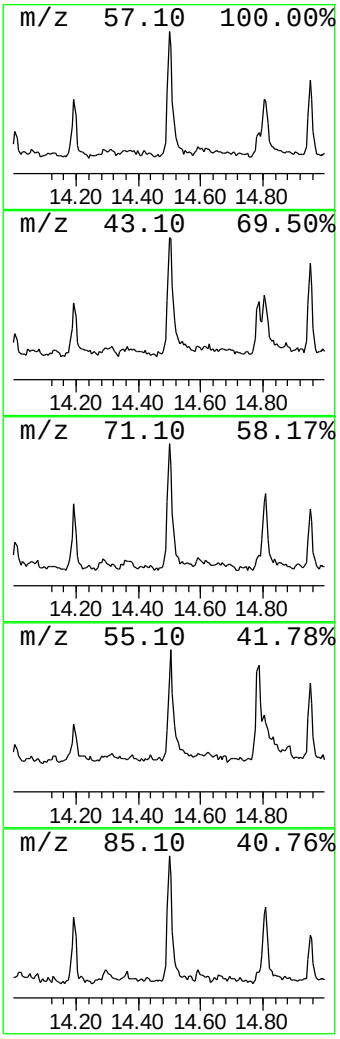
****

Peak Number 4 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.43 ng	293047	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3	Cyclopentadecane	210	C15H30	000295-48-7	90
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

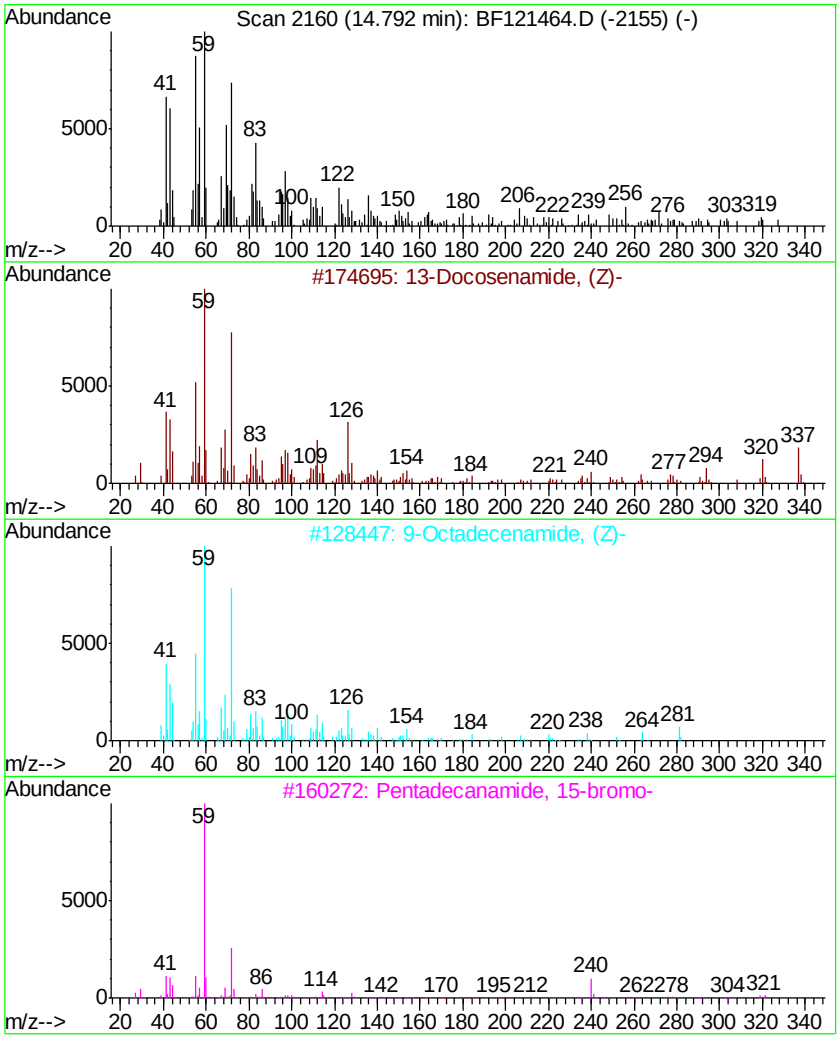
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

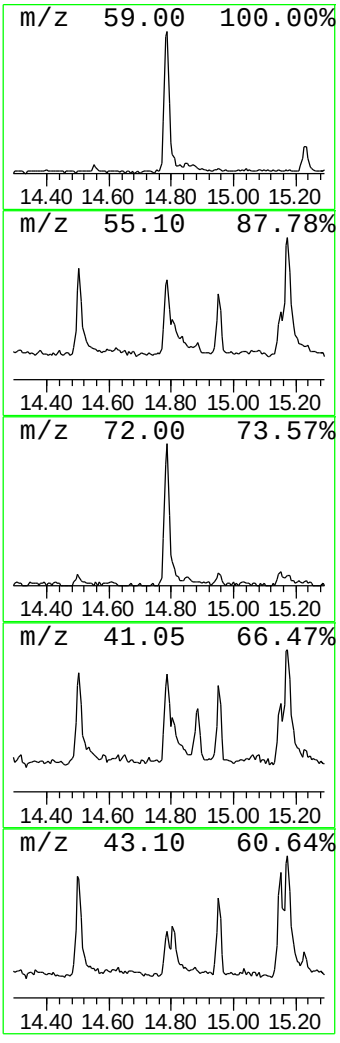
****

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.98 ng	285054	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	38
4	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38
5	Benzoic acid, 4-[3-(diethylamino...	318	C17H22N2O4	1000350-41-4	38





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

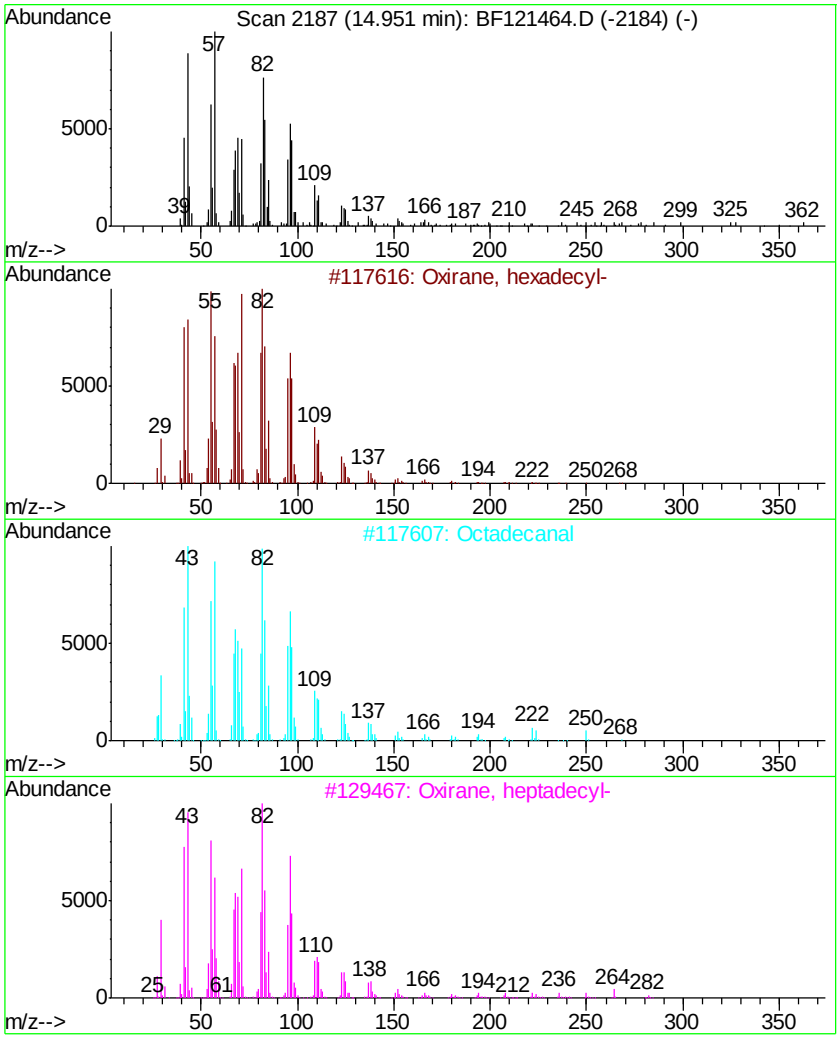
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

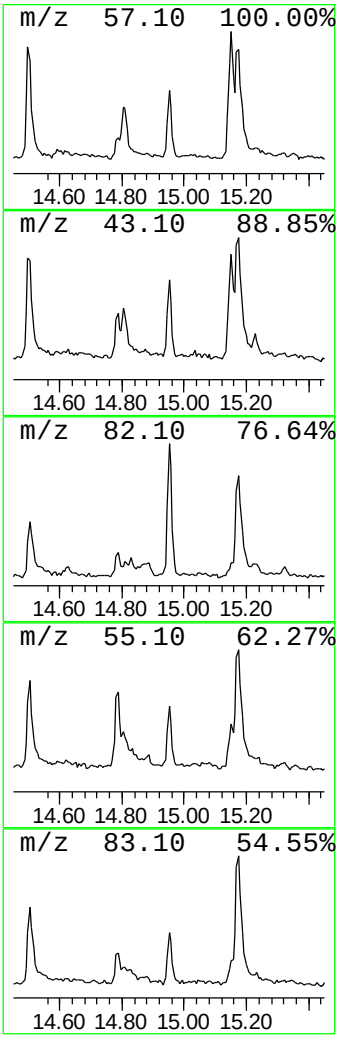
****

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.42 ng	231091	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	72
5	Pentadecanal-	226	C15H30O	002765-11-9	64





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Acq On : 28 Aug 2020 17:27
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Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

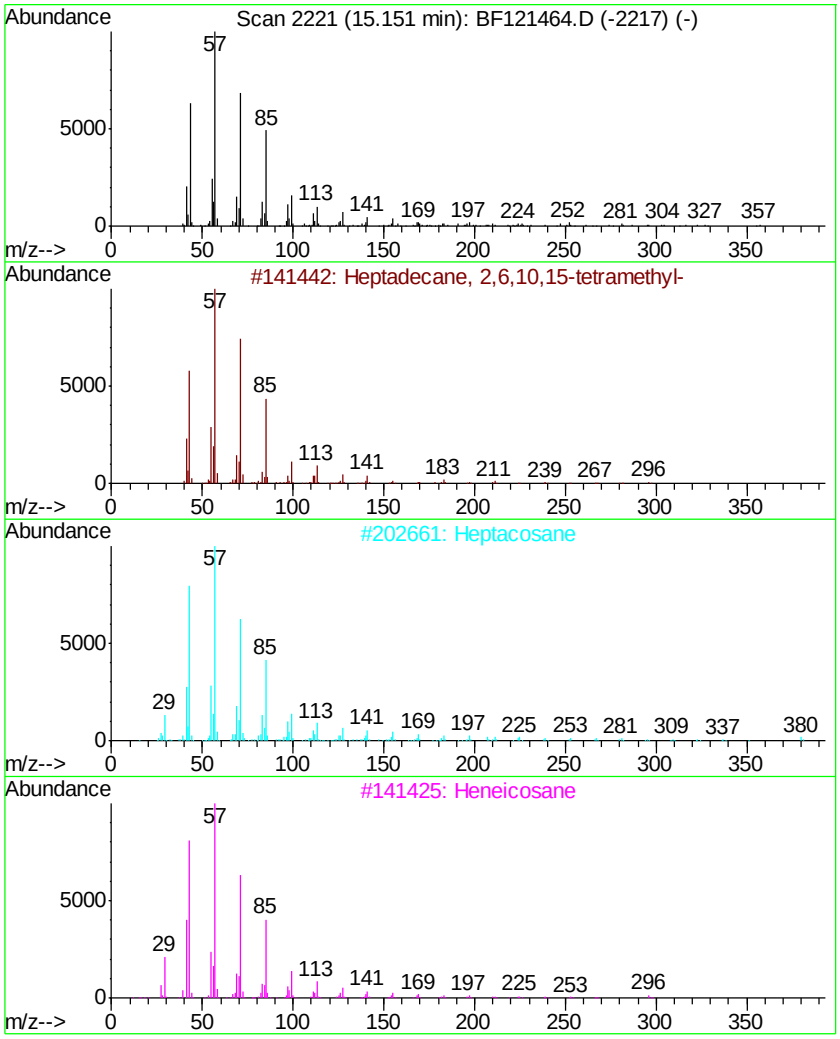
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

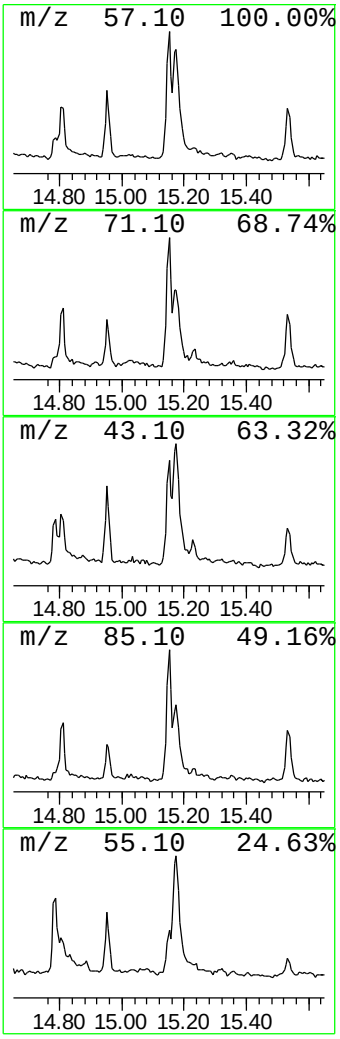
****

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.02 ng	192891	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87





Library Search Compound Report

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Data File : BF121464.D
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Operator : JU/CG
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Misc :
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Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

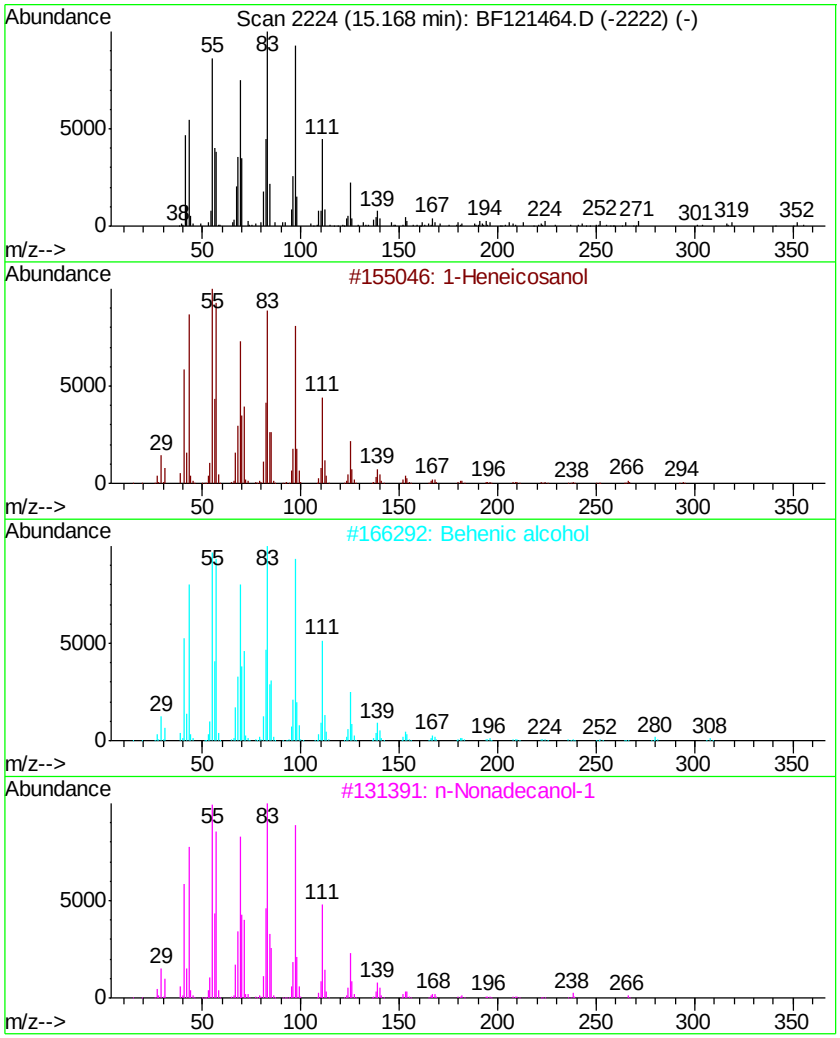
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

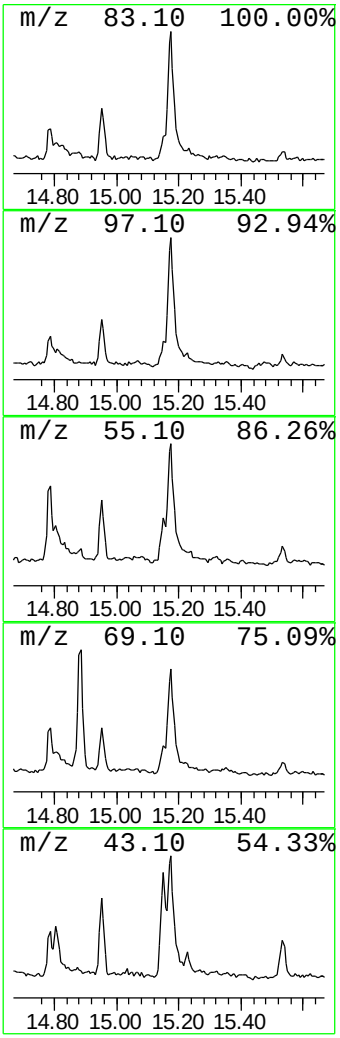
****

Peak Number 8 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	4.61 ng	440932	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	74
5	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	53





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Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
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ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.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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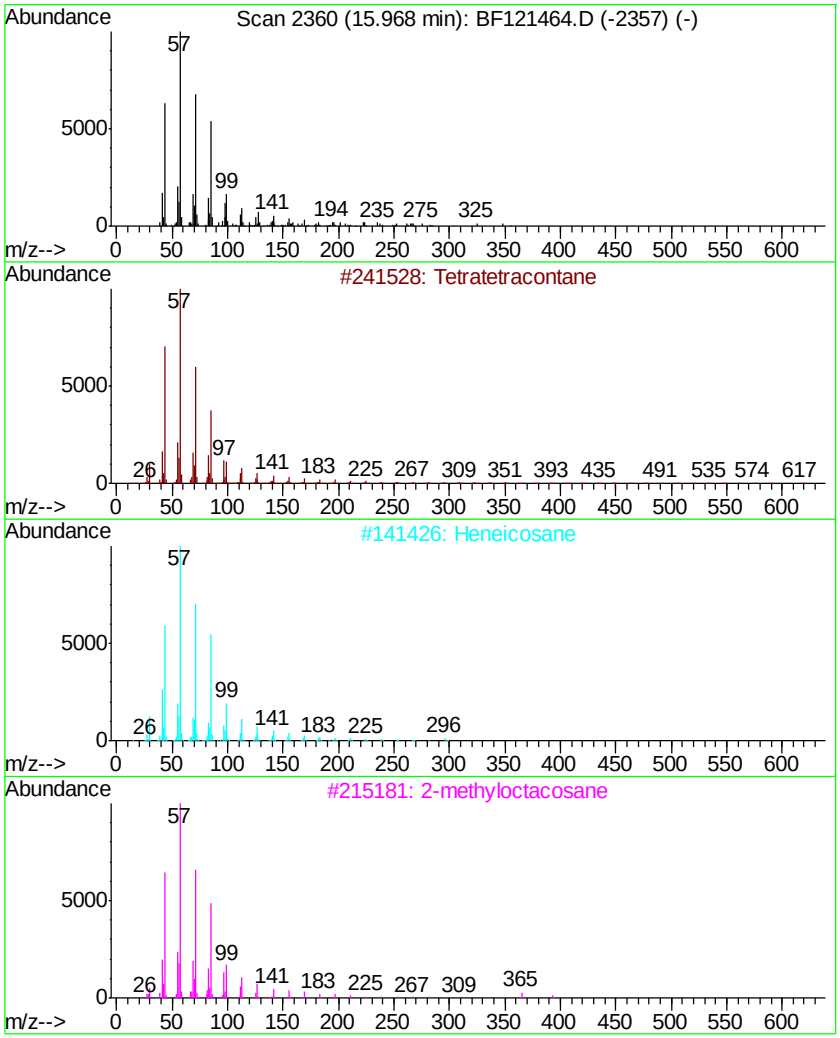
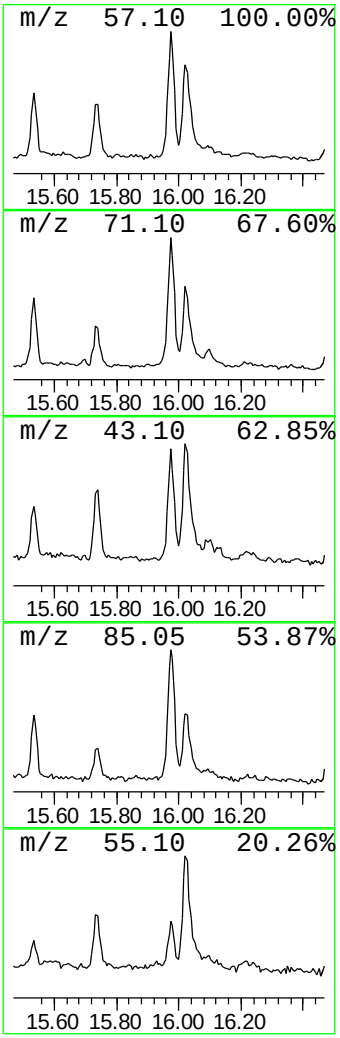
Peak Number 9 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.15 ng	205189	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hexatriacontane	507	C36H74	000630-06-8	87
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

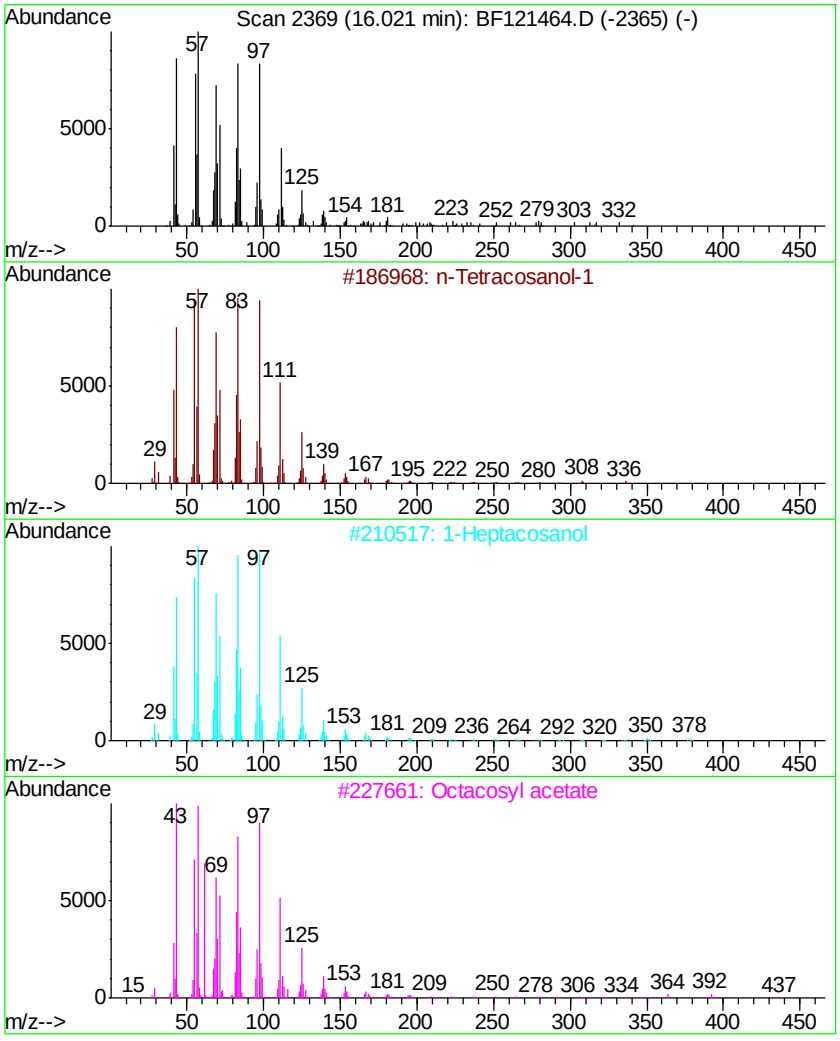
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

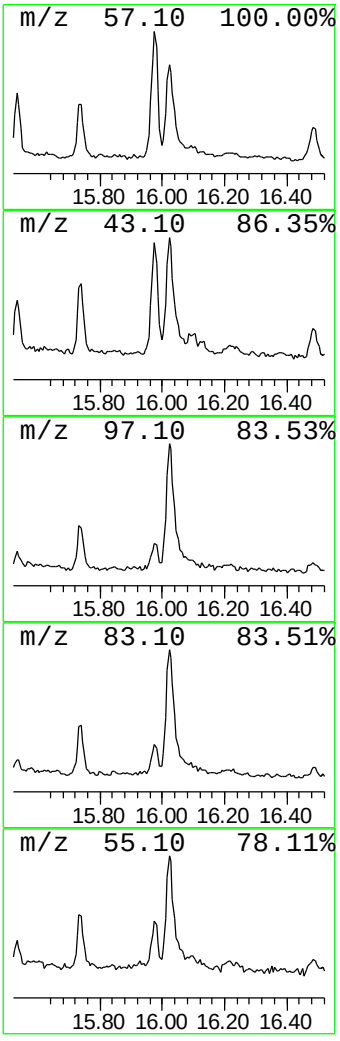
****

Peak Number 10 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.23 ng	404485	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	Octacosyl acetate	452	C30H60O2	018206-97-8	94
4	Octacosanol	410	C28H58O	000557-61-9	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082820\
Data File : BF121464.D
Acq On : 28 Aug 2020 17:27
Operator : JU/CG
Sample : L3837-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 789UMR-TP12-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082720.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...	2.16	27.0	ng	2443180	1	6.86	1809560	20.0
n-Hexadecanoic acid	11.91	3.8	ng	541905	4	11.38	2865440	20.0
5-Eicosene, (E)-	13.87	14.3	ng	1729650	5	14.02	2412010	20.0
1-Heneicosanol	14.50	2.4	ng	293047	5	14.02	2412010	20.0
13-Docosenamide, ...	14.79	3.0	ng	285054	6	15.49	1910870	20.0
Oxirane, hexadecyl-	14.95	2.4	ng	231091	6	15.49	1910870	20.0
Heptadecane, 2,6,...	15.15	2.0	ng	192891	6	15.49	1910870	20.0
Behenic alcohol	15.17	4.6	ng	440932	6	15.49	1910870	20.0
Tetratetracontane	15.97	2.1	ng	205189	6	15.49	1910870	20.0
n-Tetracosanol-1	16.02	4.2	ng	404485	6	15.49	1910870	20.0