LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

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-BF051019.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	5.451	568	572	603	rBV	3427792	4073672	92.69%	9.994%
2	6.463	740	744	762	rBV	3811650	4385568	99.79%	10.760%
3	6.592	762	766	781	rVB	4424810	4114843	93.63%	10.095%
4	6.810	800	803	813	rBV	1003067	897398	20.42%	2.202%
5	6.969	826	830	848	rBV	3473265	3052307	69.45%	7.489%
6	7.375	895	899	912	rBV	2576585	2659941	60.52%	6.526%
7	8.092	1017	1021	1039	rBV	1282478	1166572	26.54%	2.862%
8	9.169	1200	1204	1207	rBV	4795405	4122764	93.81%	10.115%
9	9.563	1267	1271	1277	rBV	523153	429801	9.78%	1.054%
10	9.845	1316	1319	1328	rVB	1476086	1280609	29.14%	3.142%
11	10.639	1450	1454	1466	rBV	2823853	2922143	66.49%	7.169%
12	11.333	1569	1572	1582	rBV	1543670	1459515	33.21%	3.581%
13	11.863	1658	1662	1671	rBV	249217	317486	7.22%	0.779%
14	12.645	1792	1795	1805	rBV6	32617	50986	1.16%	0.125%
15	12.915	1837	1841	1845	rBV	4291128	4394968	100.00%	10.783%
16	13.804	1989	1992	2004	rBV	405971	619887	14.10%	1.521%
17	13.980	2018	2022	2029	rBV	1370706	1310502	29.82%	3.215%
18	14.121	2043	2046	2054	rBV	98322	104168	2.37%	0.256%
19	14.427	2095	2098	2101	rBV	149218	146921	3.34%	0.360%
20	14.727	2145	2149	2153	rBV	212975	199686	4.54%	0.490%
21	14.804	2158	2162	2166	rBV	493819	493040	11.22%	1.210%
22	15.056	2201	2205	2209	rBV	261598	288375	6.56%	0.707%
23	15.439	2263	2270	2282	rBV3	918089	1508156	34.32%	3.700%
24	15.851	2335	2340	2346	rBV	267339	389836	8.87%	0.956%
25	16.339	2418	2423	2432	rVB2	144625	259481	5.90%	0.637%
26	16.915	2516	2521	2528	rVB3	61524	111207	2.53%	0.273%

Sum of corrected areas: 40759832

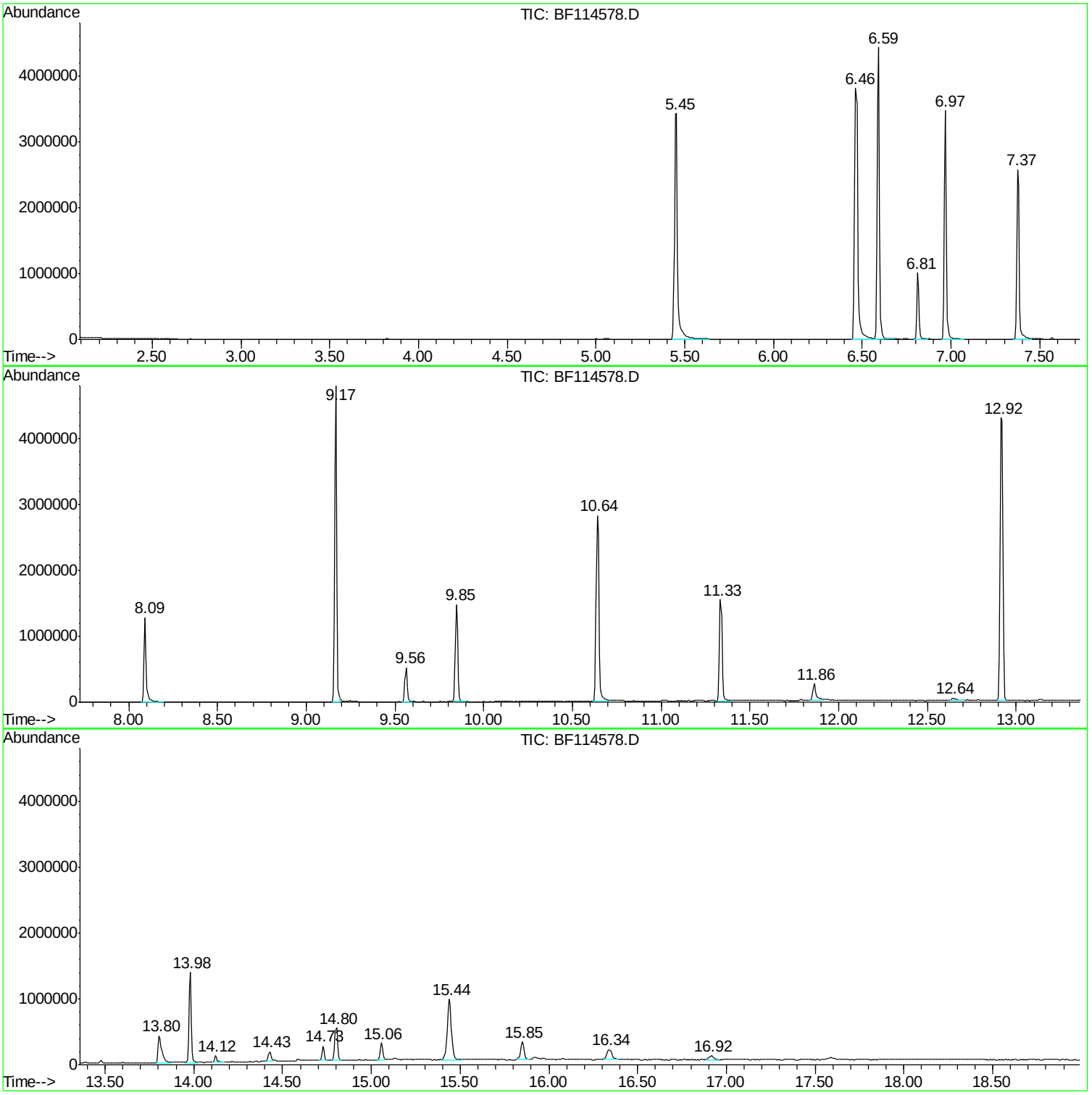
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052419\
Data File : BF114578.D
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Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

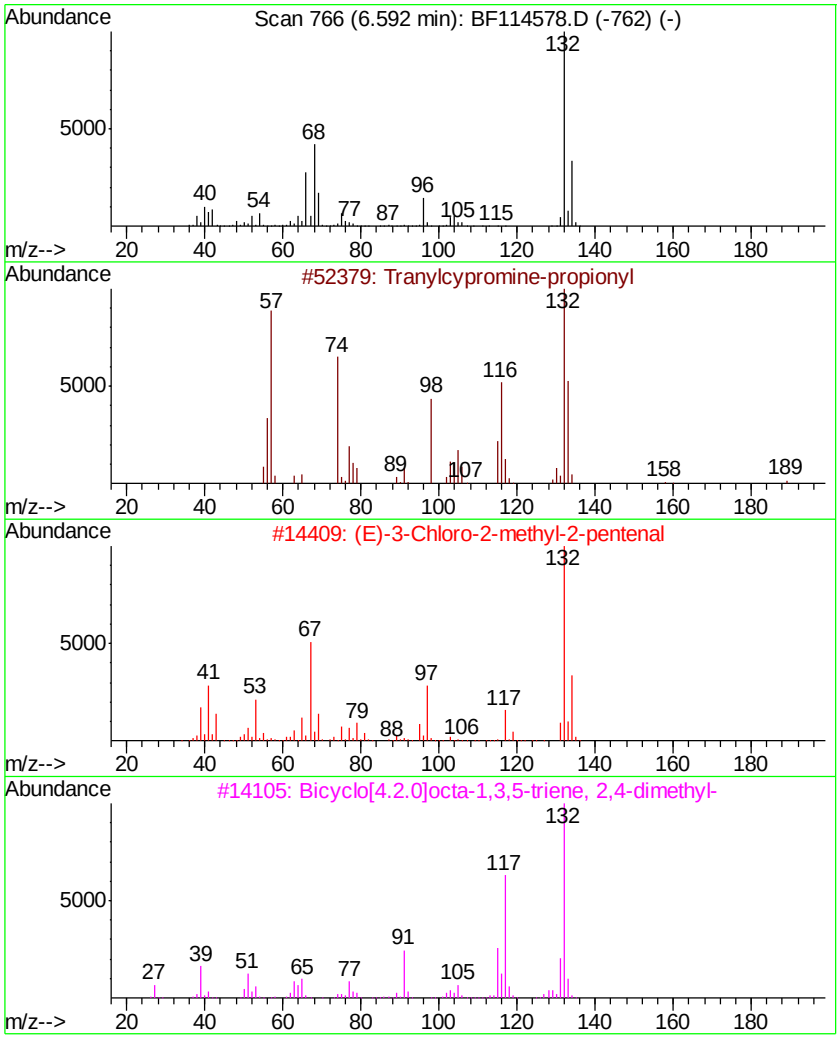
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

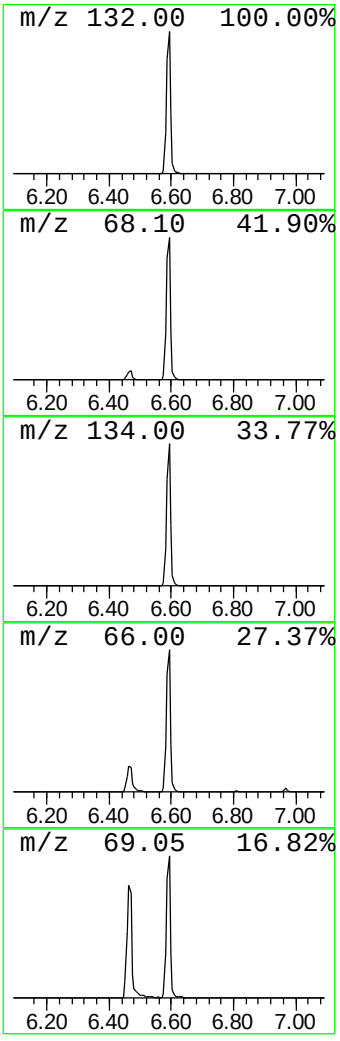
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	91.71 ng	4114840	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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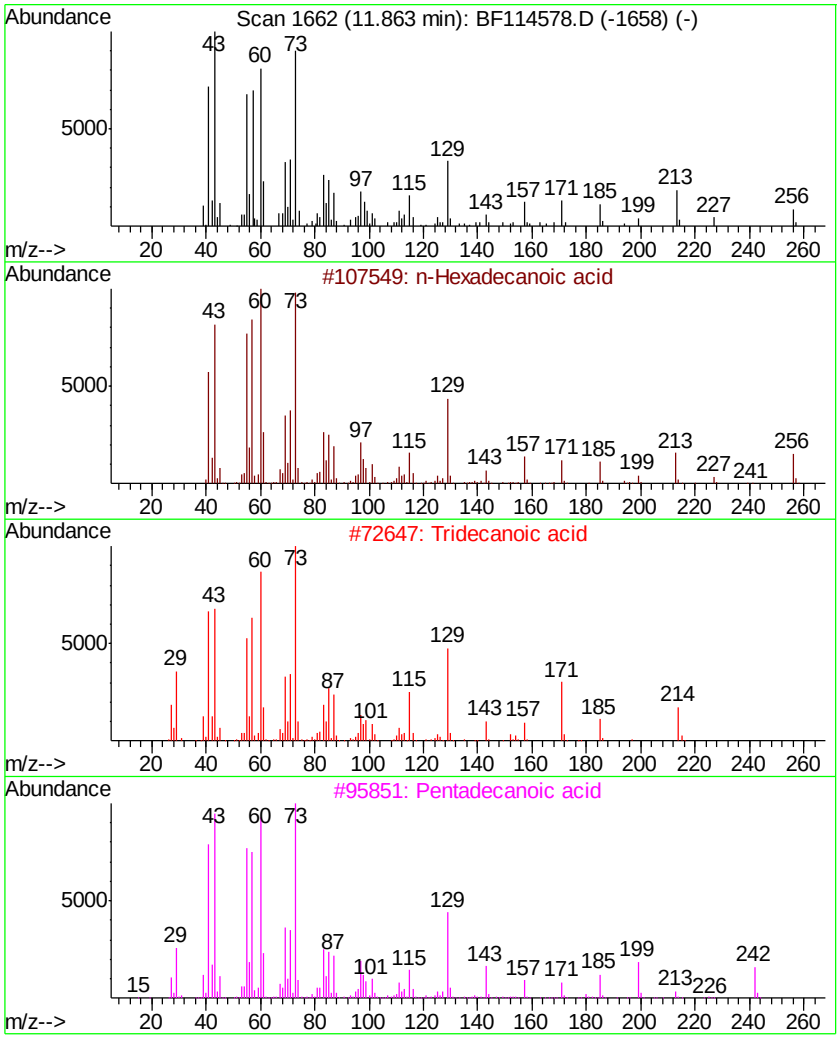
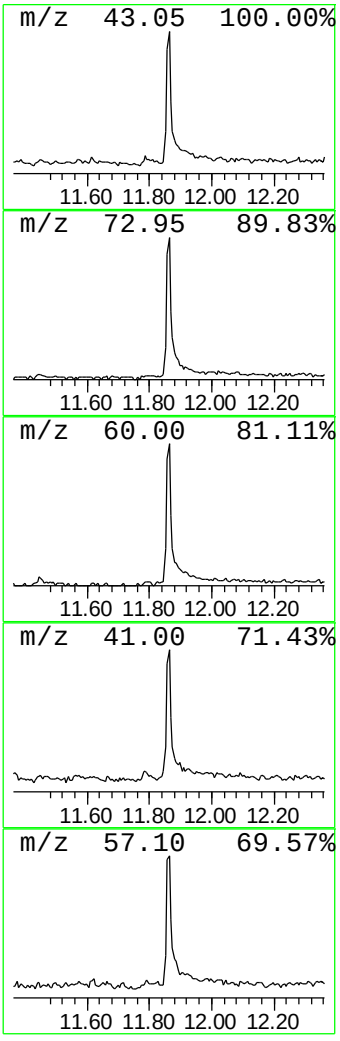
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.35 ng	317486	Phenanthrene-d10	11.33

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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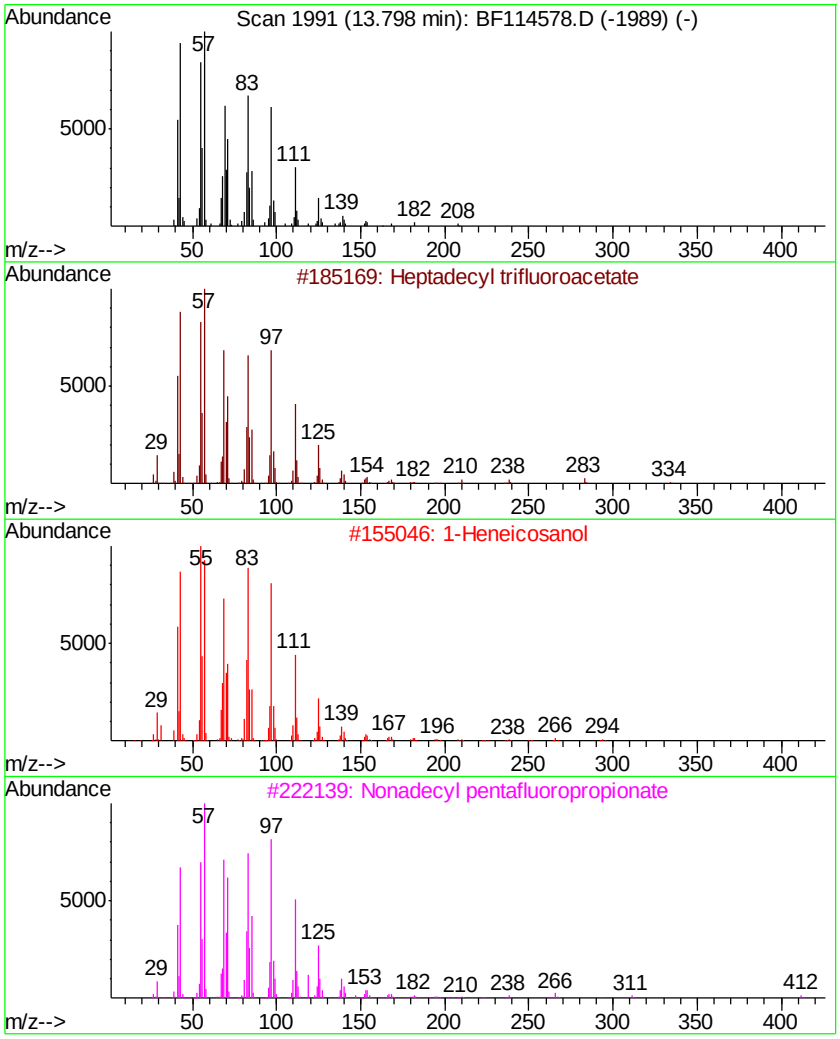
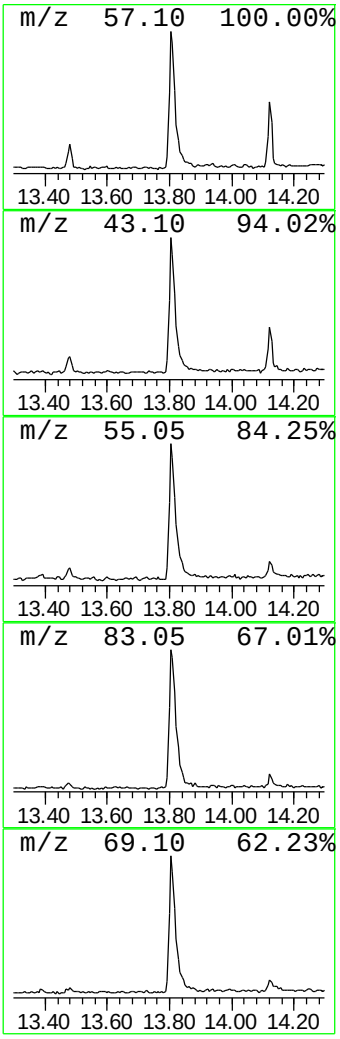
Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	9.46 ng	619887	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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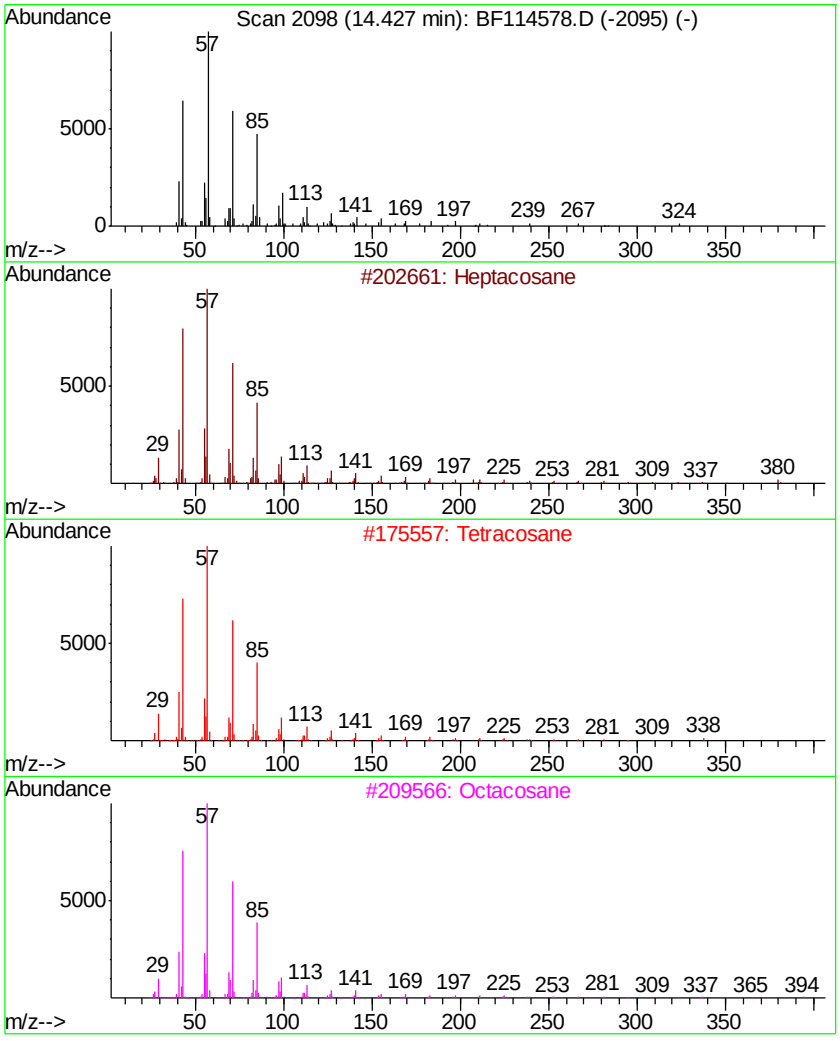
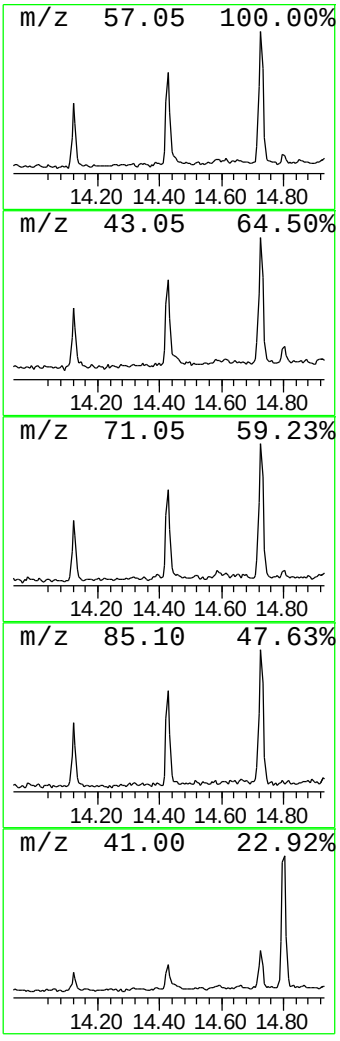
Peak Number 5 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.24 ng	146921	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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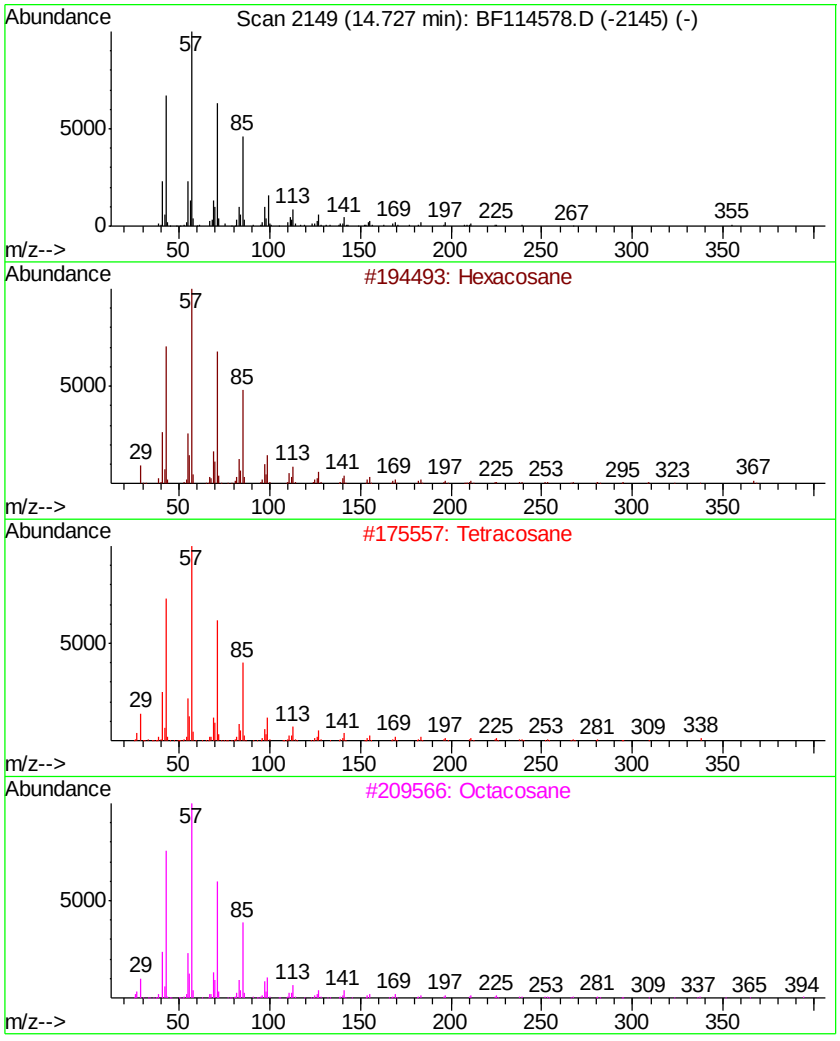
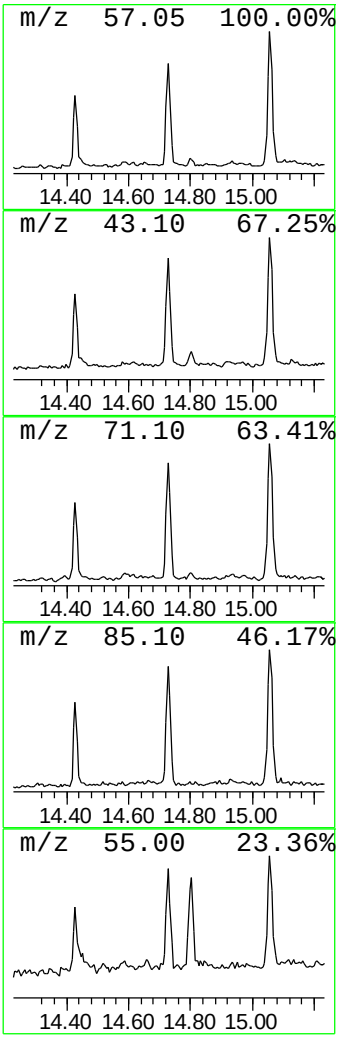
Peak Number 6 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.65 ng	199686	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
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Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

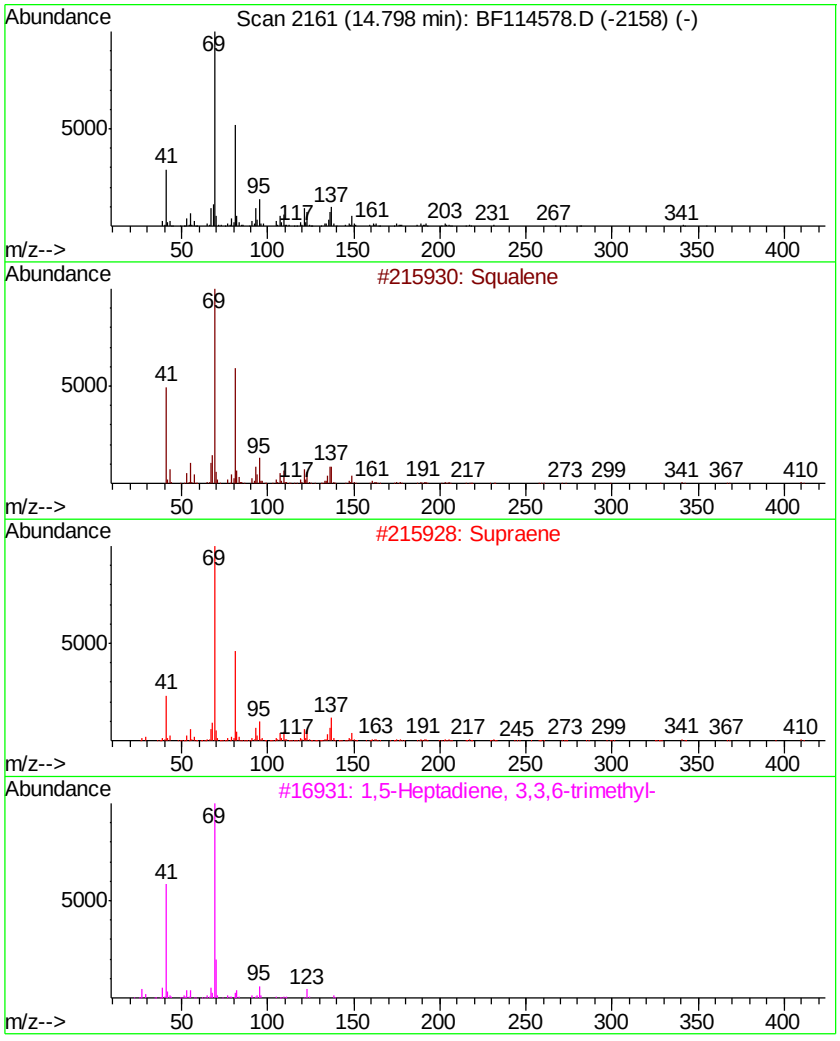
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

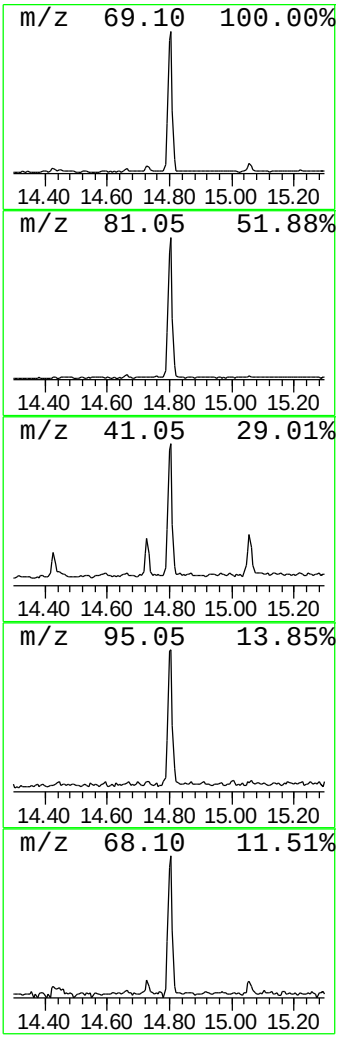
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	6.54 ng	493040	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	91
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	49





Library Search Compound Report

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Data File : BF114578.D
Acq On : 24 May 2019 19:12
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Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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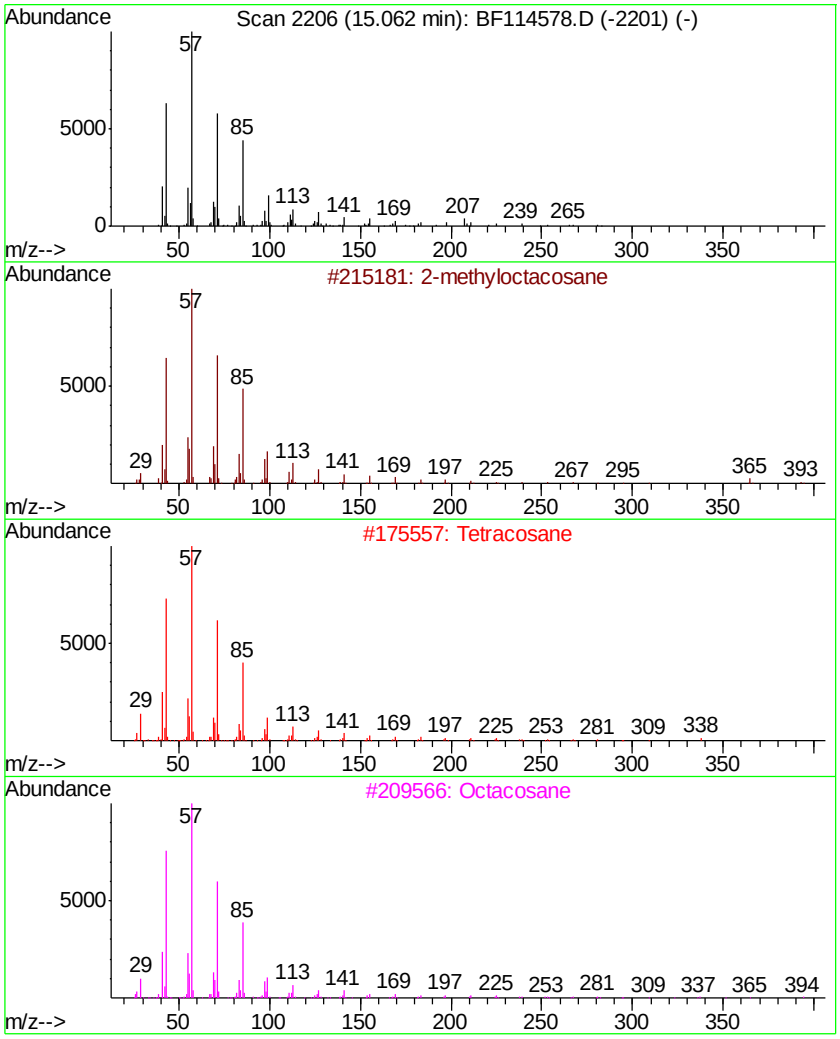
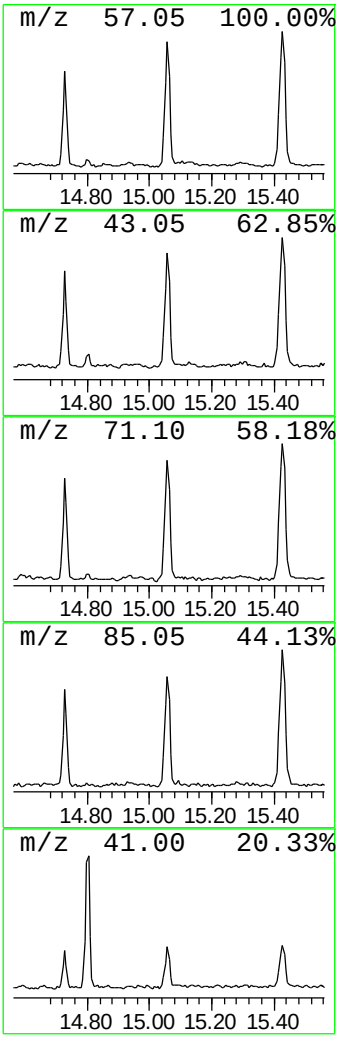
Peak Number 8 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.82 ng	288375	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Pentacosane	352	C25H52	000629-99-2	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
Operator : JU/SJ
Sample : K3019-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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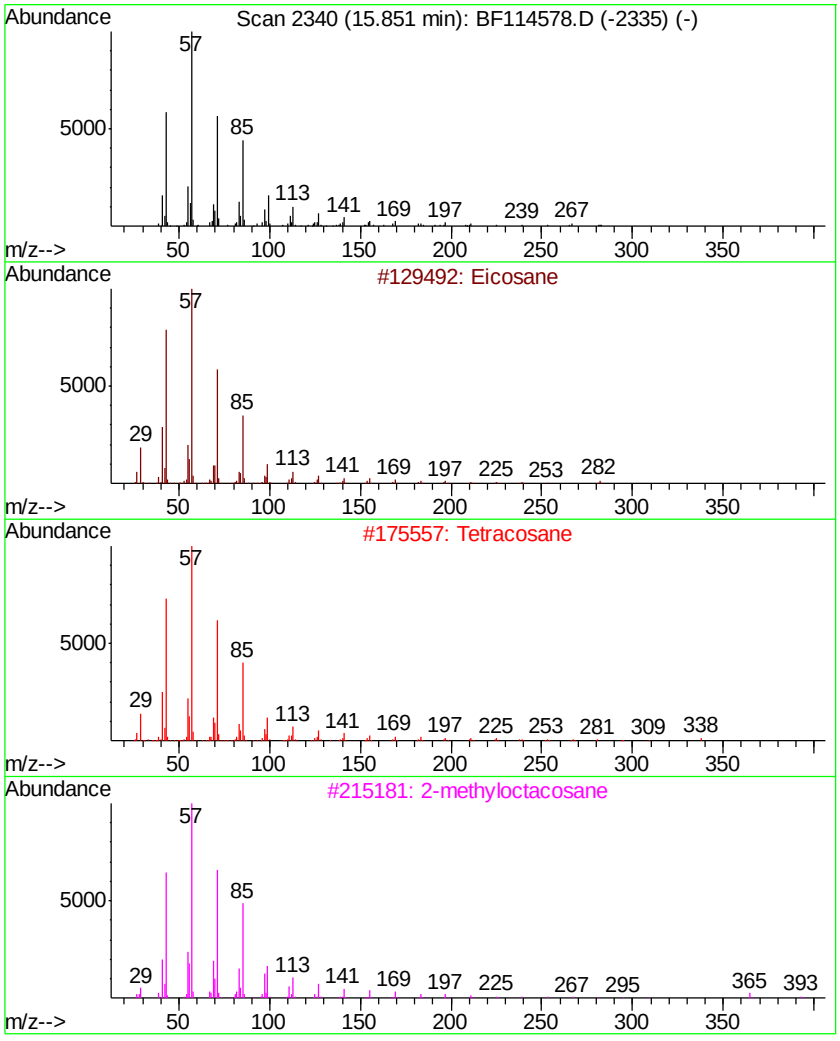
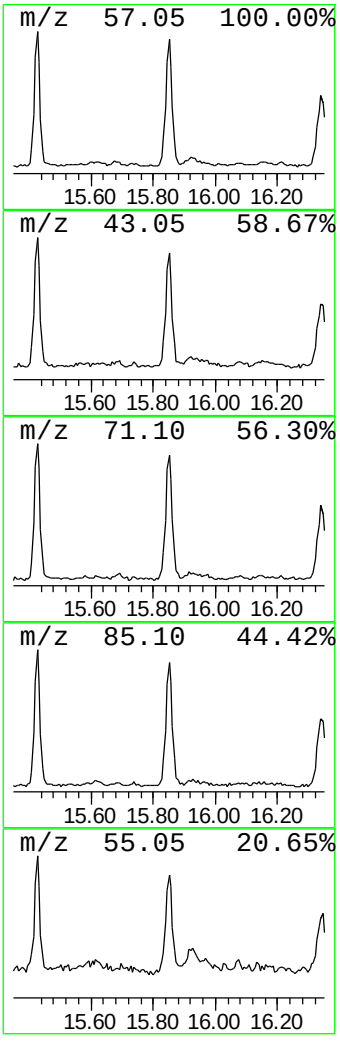
Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	5.17 ng	389836	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Tetracosane	338	C24H50	000646-31-1	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052419\
Data File : BF114578.D
Acq On : 24 May 2019 19:12
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Instrument : BNA_F
ClientSampleId : RBR200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.59	6.59	91.7	ng	4114840	1	6.81	897398	20.0
n-Hexadecanoic acid	11.86	4.3	ng	317486	4	11.33	1459520	20.0
Heptadecyl triflu...	13.80	9.5	ng	619887	5	13.98	1310500	20.0
Heptacosane	14.43	2.2	ng	146921	5	13.98	1310500	20.0
Hexacosane	14.73	2.6	ng	199686	6	15.44	1508160	20.0
Squalene	14.80	6.5	ng	493040	6	15.44	1508160	20.0
2-methyloctacosane	15.06	3.8	ng	288375	6	15.44	1508160	20.0
Eicosane	15.85	5.2	ng	389836	6	15.44	1508160	20.0