LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114242.D
Acq On : 13 May 2019 21:03
Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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	2.116	3	5	19	rVB	1200777	1352700	26.43%	2.631%
2	5.498	575	580	597	rBV	4807599	5003139	97.77%	9.733%
3	6.510	747	752	755	rBV	5155384	5117267	100.00%	9.955%
4	6.633	769	773	777	rBV	5403081	5007622	97.86%	9.741%
5	6.857	807	811	814	rBV	1575481	1342928	26.24%	2.612%
6	7.010	833	837	841	rBV	3770675	3631644	70.97%	7.065%
7	7.416	902	906	909	rBV	3352946	3139089	61.34%	6.106%
8	8.133	1025	1028	1046	rVB	1762780	1678766	32.81%	3.266%
9	9.210	1207	1211	1222	rBV	5542021	5019130	98.08%	9.764%
10	9.604	1274	1278	1283	rBV	863695	779914	15.24%	1.517%
11	9.892	1323	1327	1340	rVB	1981390	1810788	35.39%	3.523%
12	10.680	1457	1461	1471	rBV	3280943	3238089	63.28%	6.299%
13	11.374	1575	1579	1583	rBV	1876276	1769970	34.59%	3.443%
14	11.904	1665	1669	1677	rBV	942704	975341	19.06%	1.897%
15	12.457	1760	1763	1766	rBV	74605	62132	1.21%	0.121%
16	12.686	1798	1802	1809	rBV	272211	351037	6.86%	0.683%
17	12.957	1844	1848	1852	rBV	4247455	4003290	78.23%	7.788%
18	13.186	1884	1887	1890	rVB	106597	109982	2.15%	0.214%
19	13.527	1942	1945	1948	rVB	125769	113437	2.22%	0.221%
20	13.851	1996	2000	2006	rBV	1018850	1129242	22.07%	2.197%
21	14.021	2025	2029	2034	rBV	1480950	1388242	27.13%	2.701%
22	14.174	2052	2055	2062	rVB	315338	301914	5.90%	0.587%
23	14.486	2105	2108	2115	rBV2	491283	722683	14.12%	1.406%
24	14.798	2158	2161	2165	rVB	465928	435679	8.51%	0.848%
25	15.133	2215	2218	2222	rBV	559004	659165	12.88%	1.282%
26	15.509	2278	2282	2290	rVB2	1337087	1801072	35.20%	3.504%
27	15.951	2354	2357	2362	rVB	325072	462036	9.03%	0.899%

Sum of corrected areas: 51406298

LSC Report - Integrated Chromatogram

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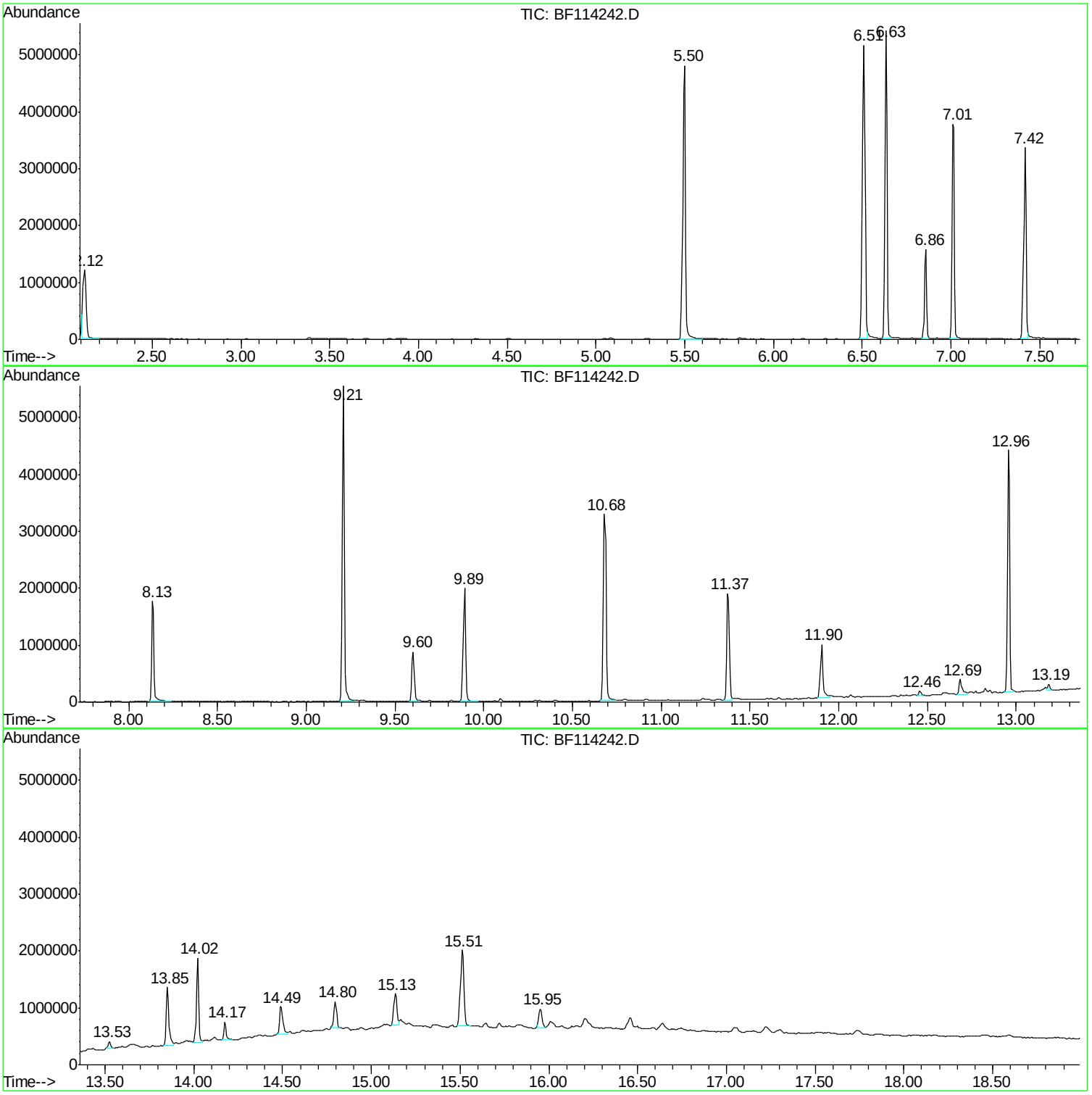
Data File : BF114242.D
Acq On : 13 May 2019 21:03
Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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

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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

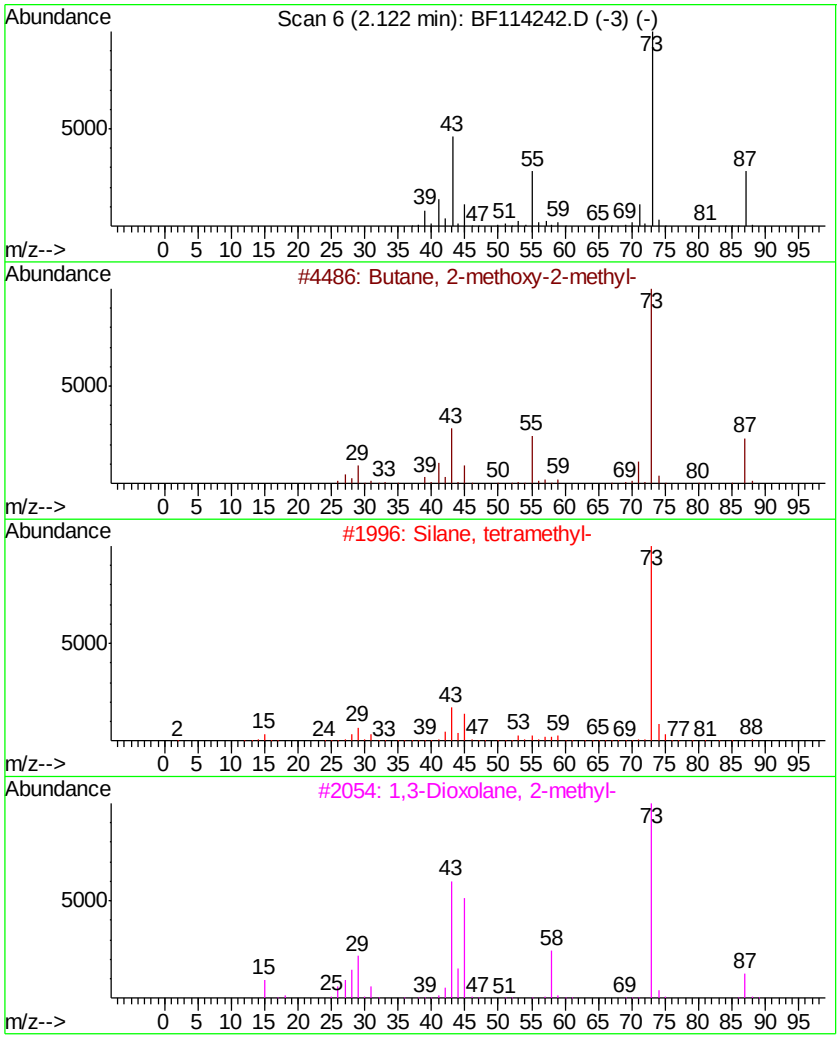
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

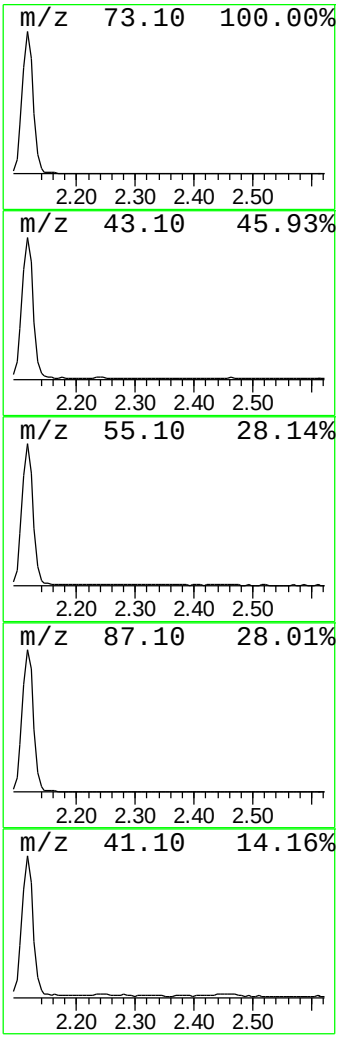
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	20.15 ng	1352700	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	56
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BF114242.D
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Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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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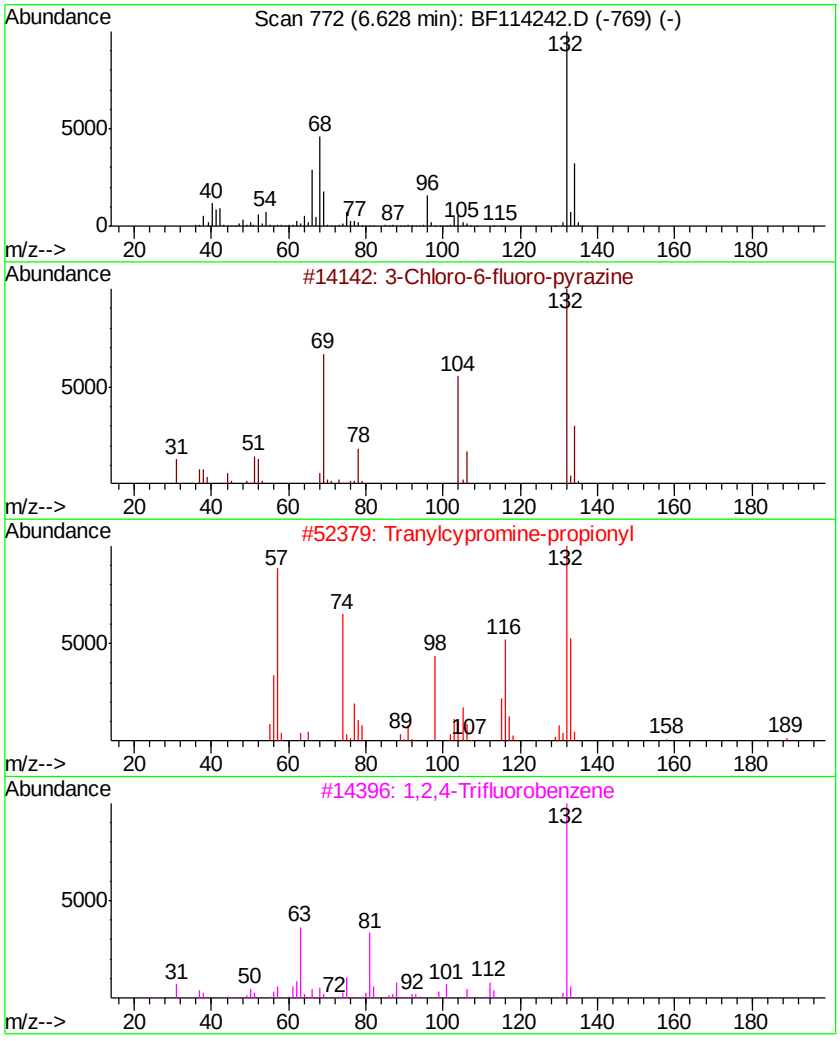
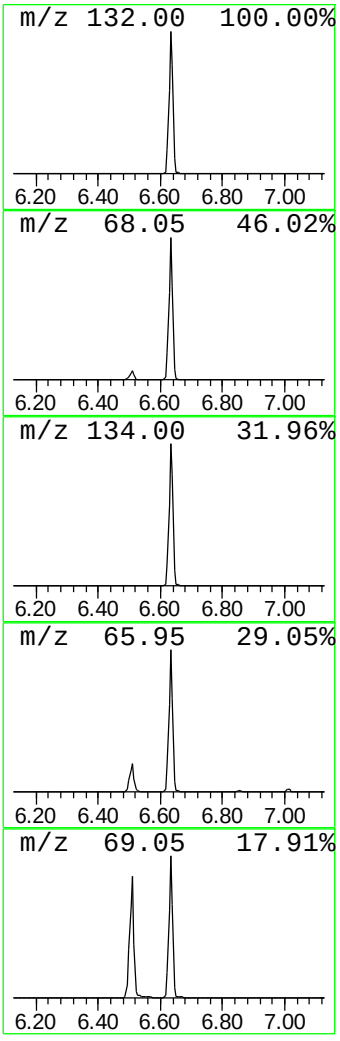
Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	74.58 ng	5007620	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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

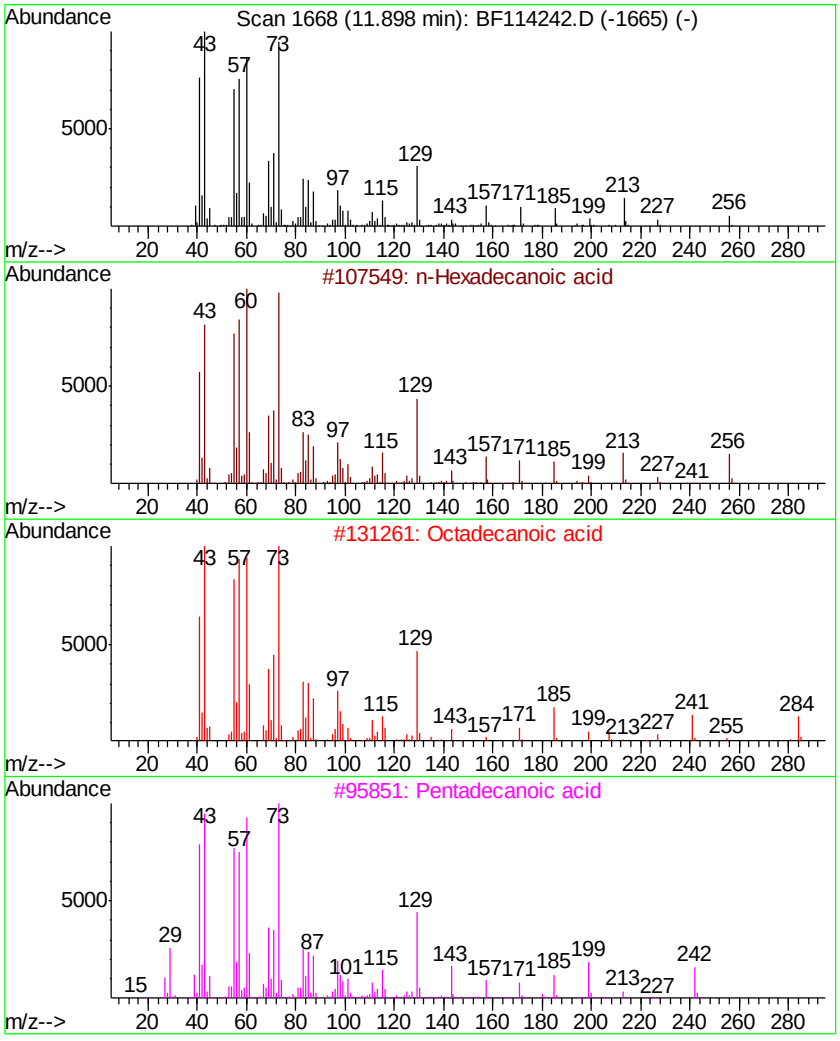
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

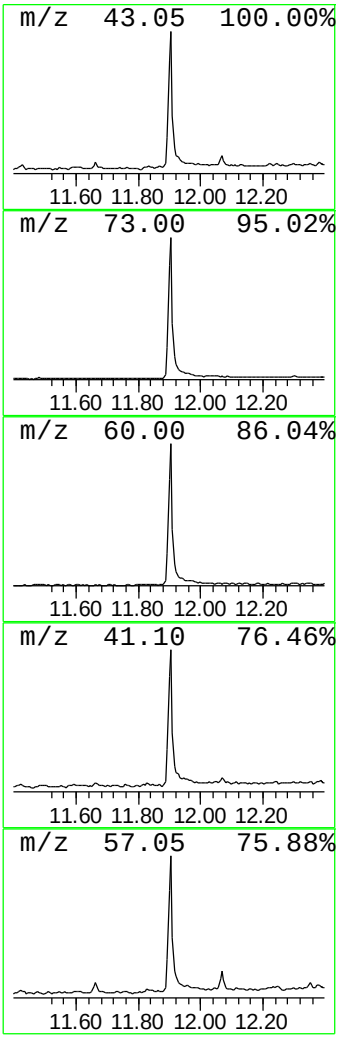
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	11.02 ng	975341	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051319\
Data File : BF114242.D
Acq On : 13 May 2019 21:03
Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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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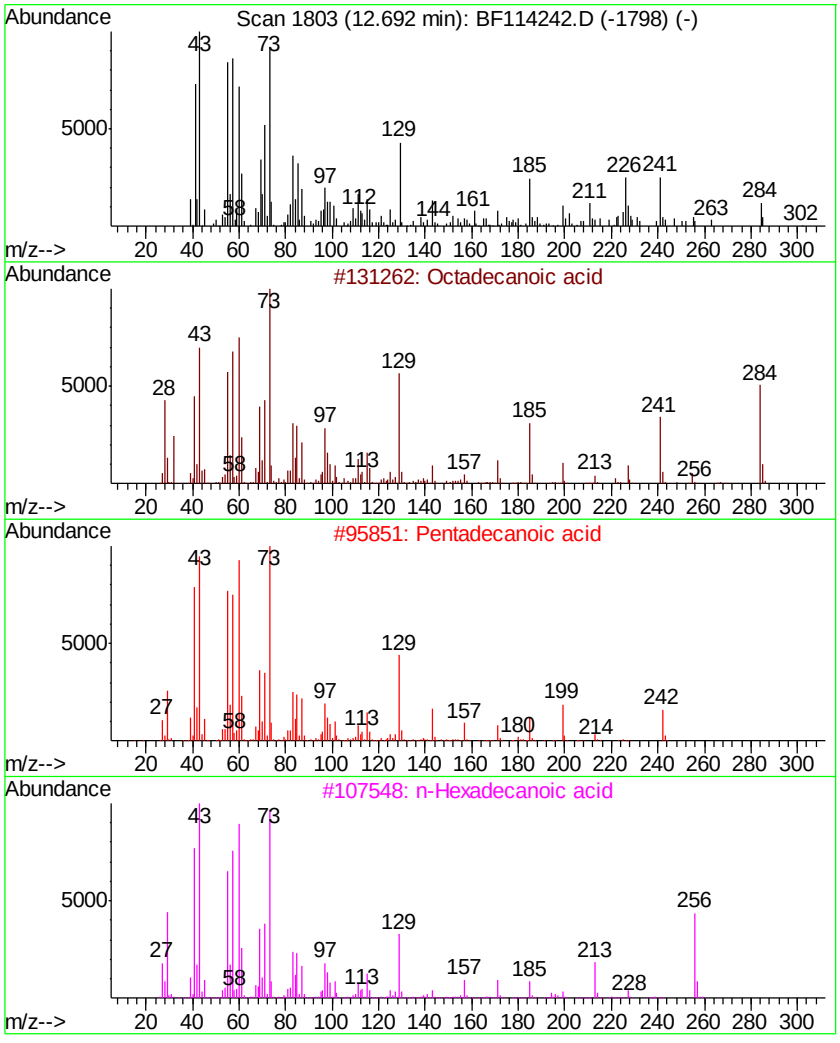
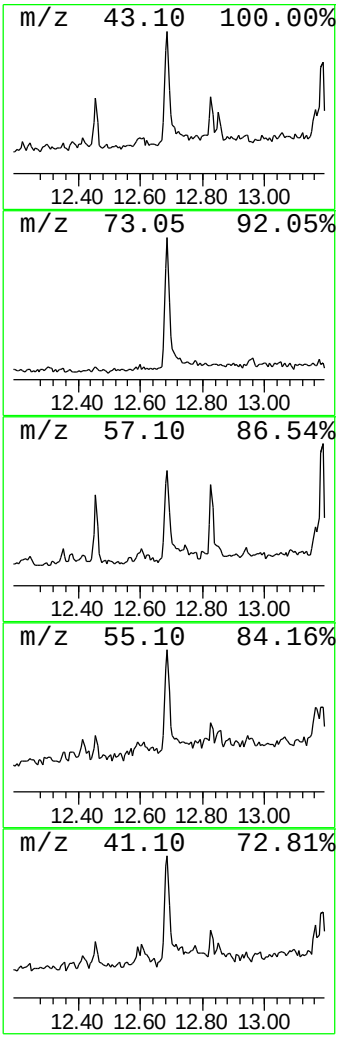
Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	3.97 ng	351037	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Hexadecane	226	C16H34	000544-76-3	25





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 11-B

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

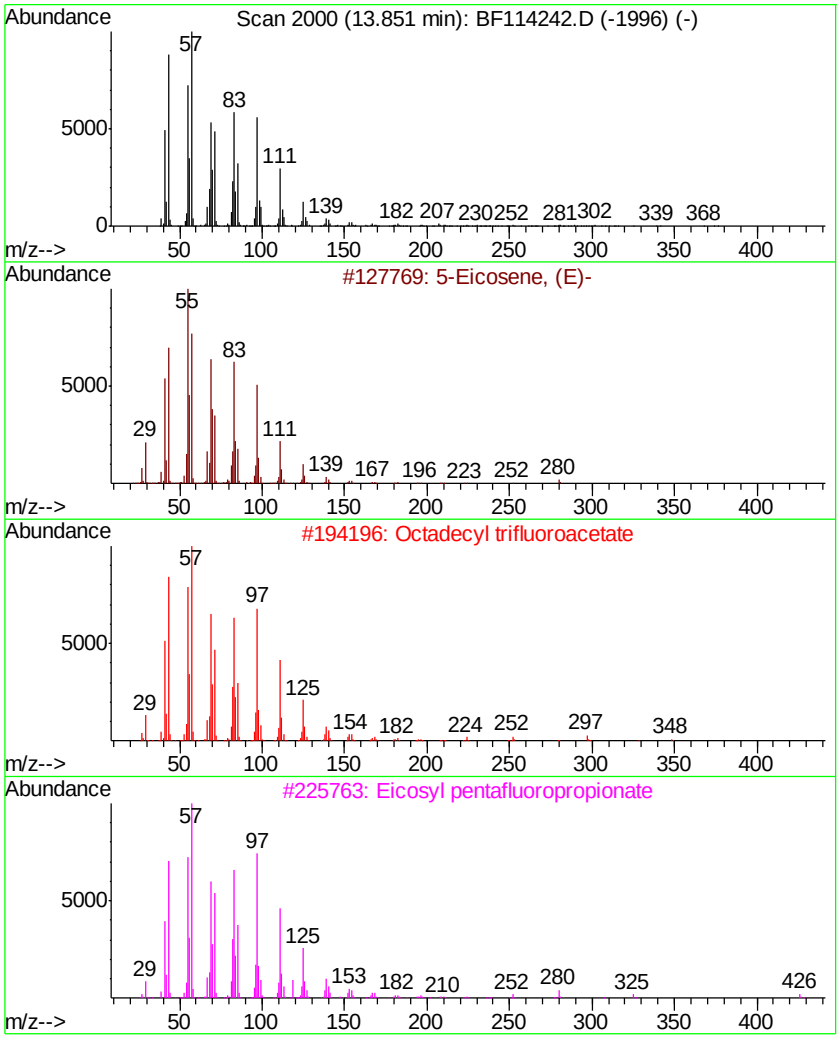
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

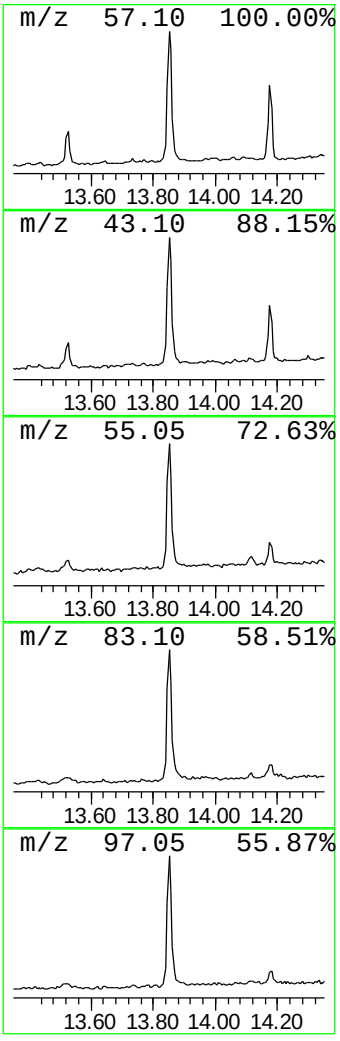
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	16.27 ng	1129240	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Library Search Compound Report

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Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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

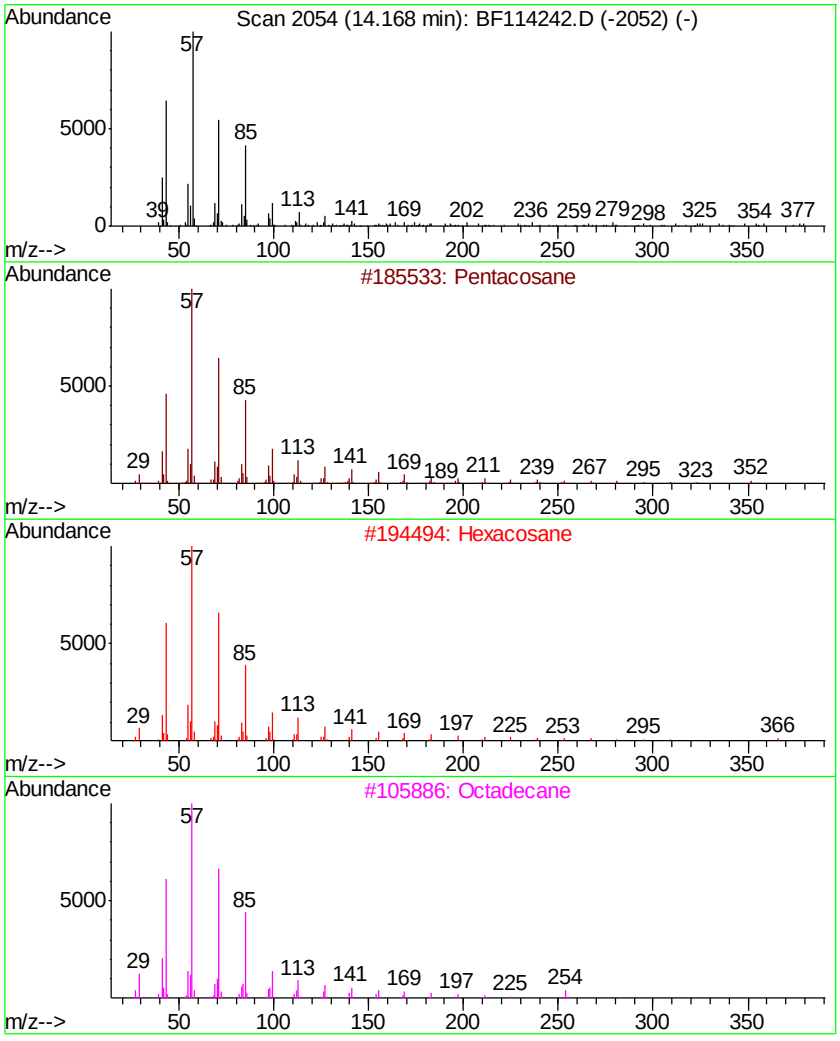
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

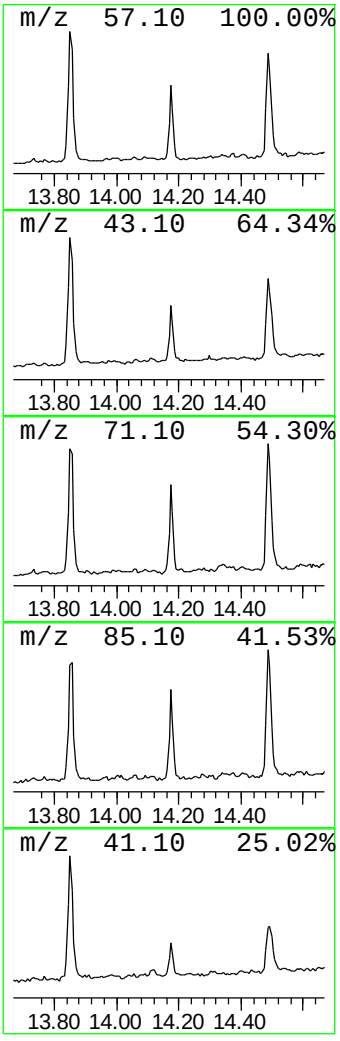
****

Peak Number 7 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	4.35 ng	301914	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	97
2	Hexacosane	366	C26H54	000630-01-3	95
3	Octadecane	254	C18H38	000593-45-3	94
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5	Heptacosane	380	C27H56	000593-49-7	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 11-B

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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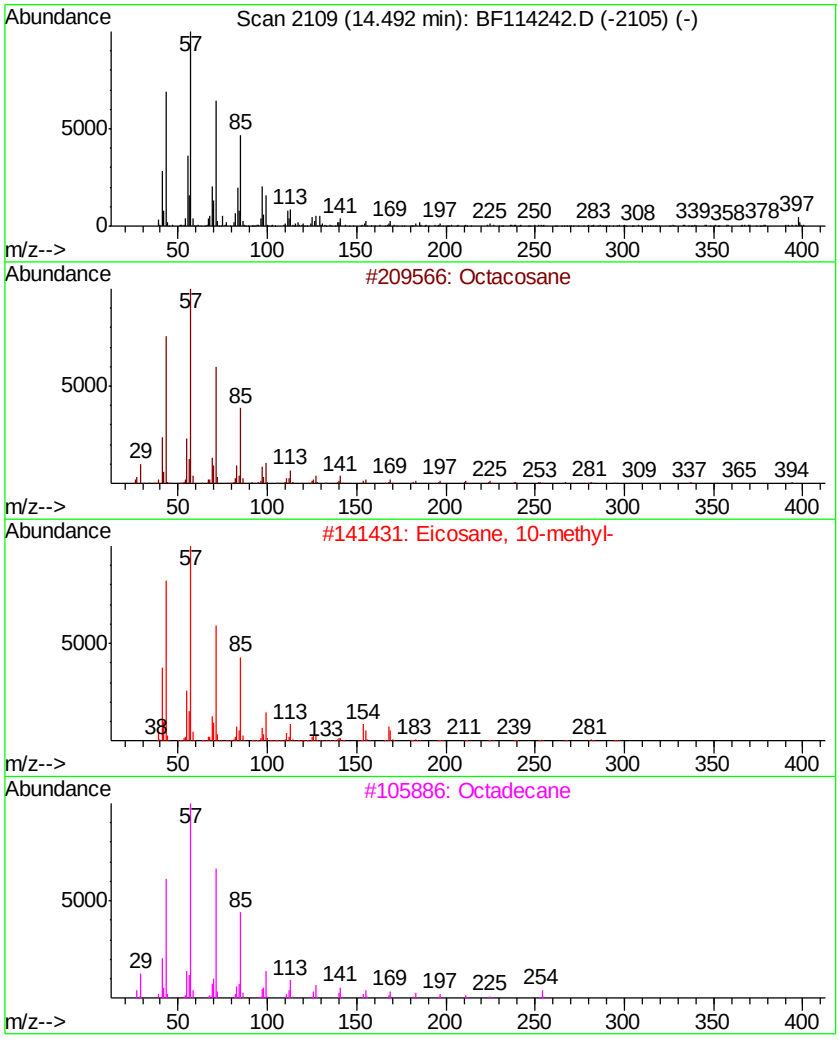
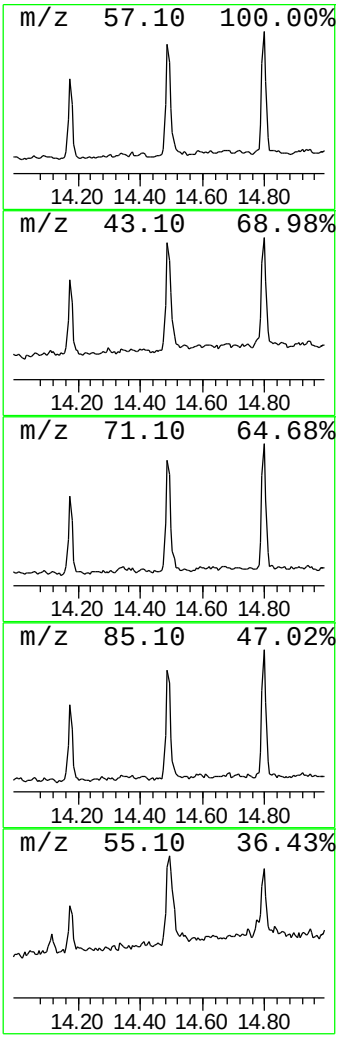
Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	10.41 ng	722683	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	98
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Octadecane	254	C18H38	000593-45-3	91
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	91
5	Hexacosane	366	C26H54	000630-01-3	90





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TIC Library : C:\DATABASE\NIST11.L
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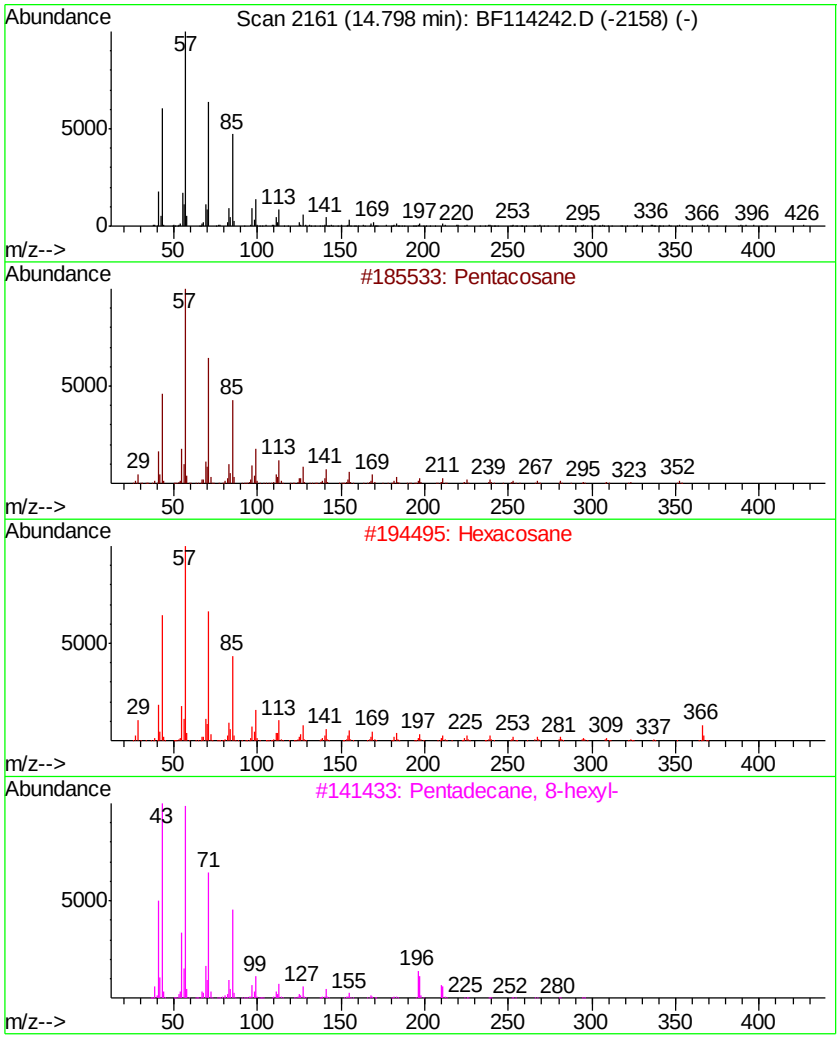
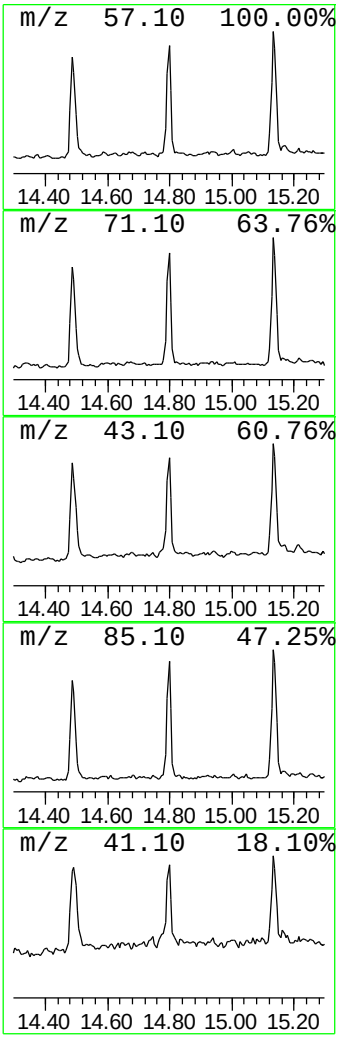
Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.84 ng	435679	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	96
2	Hexacosane	366	C26H54	000630-01-3	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4	Octadecane	254	C18H38	000593-45-3	93
5	Heptacosane	380	C27H56	000593-49-7	91





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Instrument : BNA_F
ClientSampleId : 11-B

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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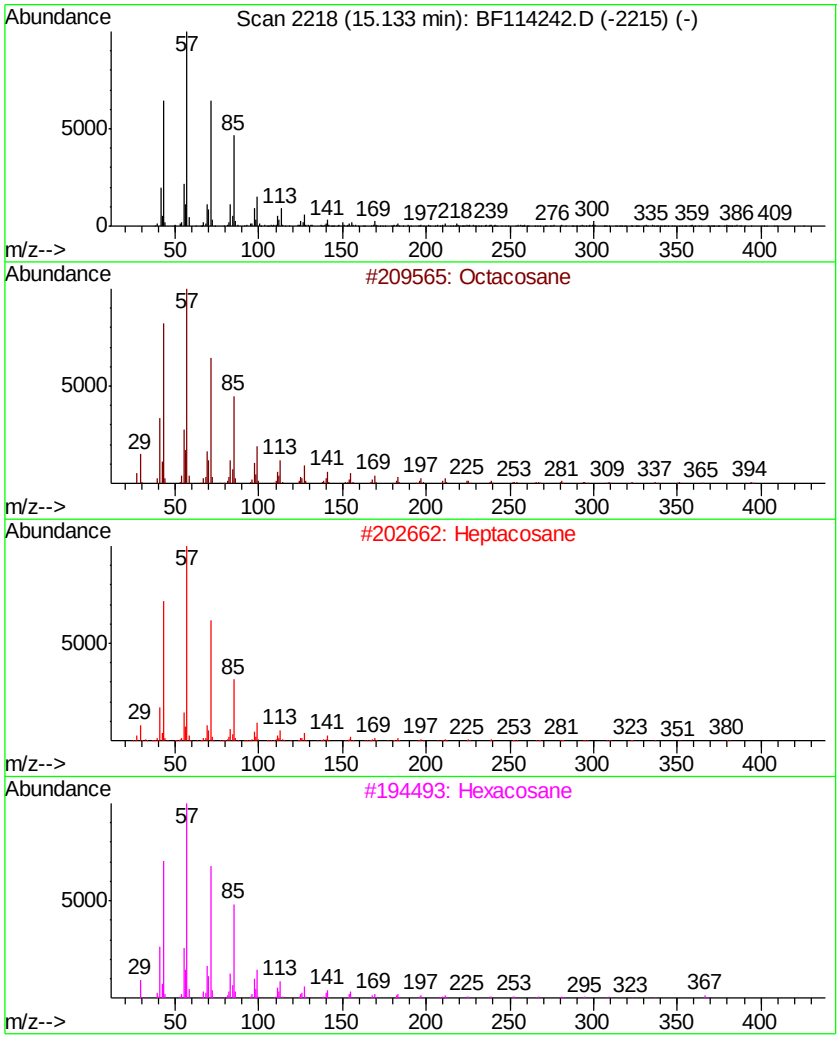
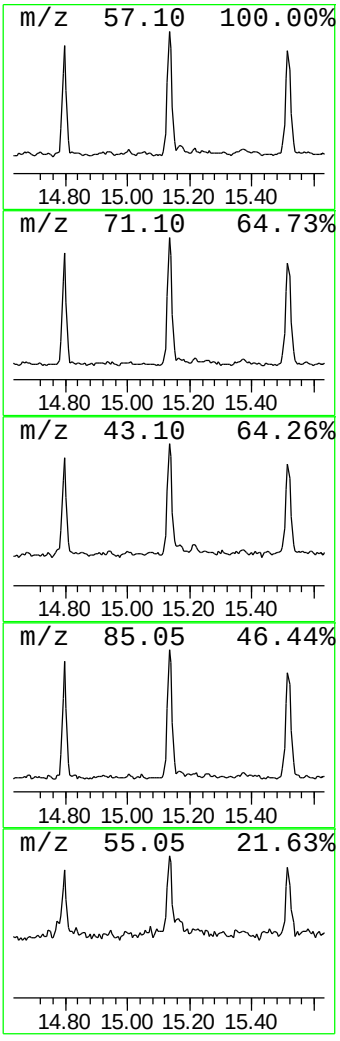
Peak Number 10 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	7.32 ng	659165	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Nonadecane	268	C19H40	000629-92-5	87





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Data File : BF114242.D
Acq On : 13 May 2019 21:03
Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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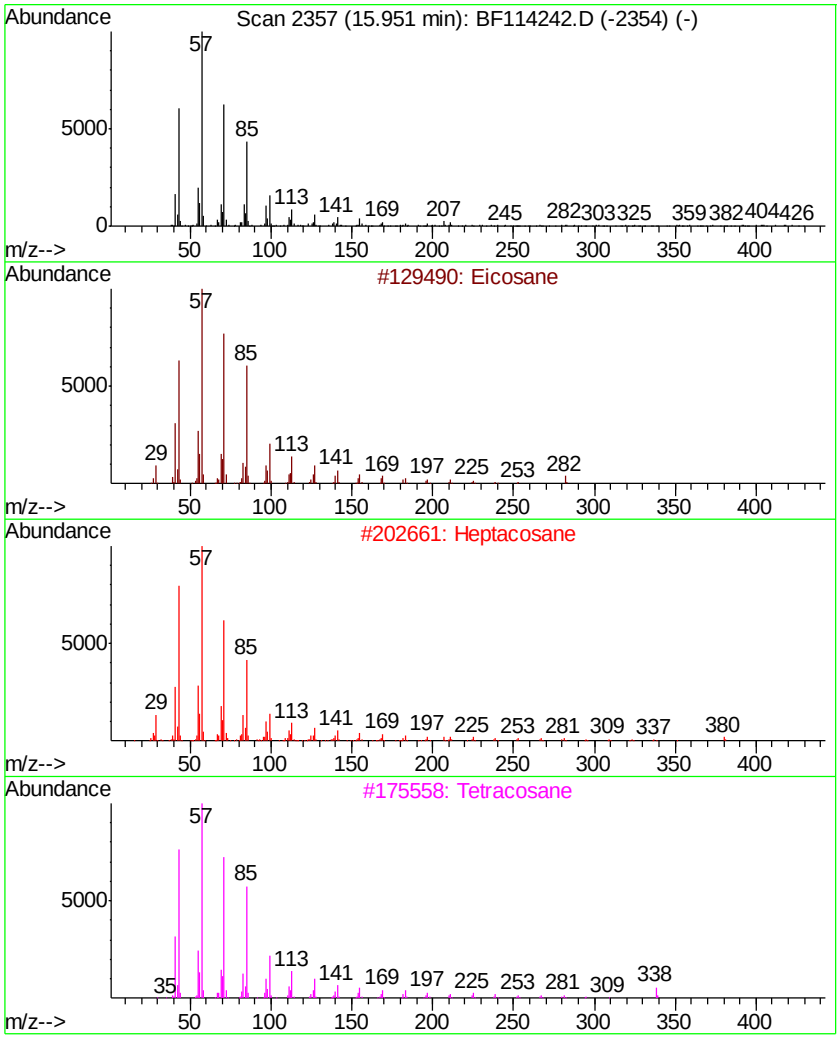
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

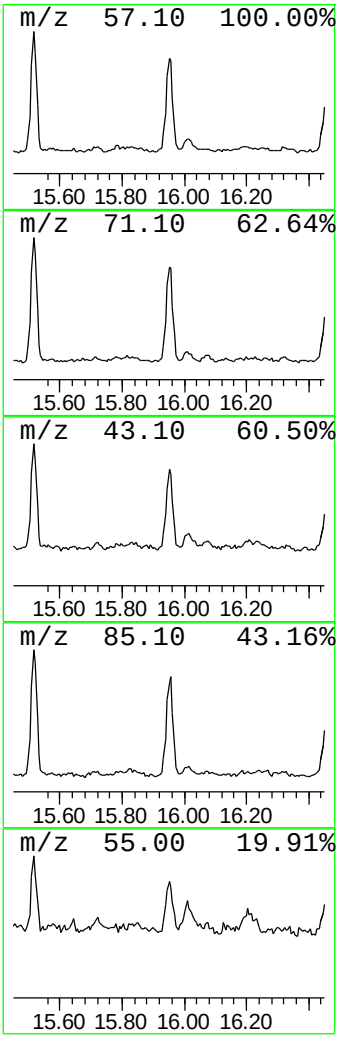
****

Peak Number 11 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	5.13 ng	462036	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptacosane	380	C27H56	000593-49-7	93
3	Tetracosane	338	C24H50	000646-31-1	93
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051319\
Data File : BF114242.D
Acq On : 13 May 2019 21:03
Operator : JU/SJ
Sample : K2823-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11-B

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
Butane, 2-methoxy...	2.12	20.1	ng	1352700	1	6.86	1342930	20.0
unknown6.63	6.63	74.6	ng	5007620	1	6.86	1342930	20.0
n-Hexadecanoic acid	11.90	11.0	ng	975341	4	11.37	1769970	20.0
Octadecanoic acid	12.69	4.0	ng	351037	4	11.37	1769970	20.0
5-Eicosene, (E)-	13.85	16.3	ng	1129240	5	14.02	1388240	20.0
Pentacosane	14.17	4.3	ng	301914	5	14.02	1388240	20.0
Octacosane	14.49	10.4	ng	722683	5	14.02	1388240	20.0
Hexacosane	14.80	4.8	ng	435679	6	15.51	1801070	20.0
Heptacosane	15.13	7.3	ng	659165	6	15.51	1801070	20.0
Eicosane	15.95	5.1	ng	462036	6	15.51	1801070	20.0