LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

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-BF022719.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	5.351	550	555	571	rBV	3068680	3096039	89.16%	8.707%
2	6.022	666	669	673	rBV	72191	64457	1.86%	0.181%
3	6.375	724	729	739	rBV	3007751	3305355	95.19%	9.296%
4	6.510	747	752	755	rBV	3650069	3324203	95.74%	9.349%
5	6.739	787	791	795	rBV	1313848	1033153	29.75%	2.906%
6	6.898	814	818	821	rBV	3000987	2611884	75.22%	7.346%
7	7.298	881	886	889	rBV	2124243	1986079	57.20%	5.586%
8	8.022	1005	1009	1028	rBV	1263690	1253522	36.10%	3.525%
9	9.098	1188	1192	1206	rBV	3796321	3472264	100.00%	9.765%
10	9.486	1255	1258	1265	rBV	153850	158561	4.57%	0.446%
11	9.769	1302	1306	1316	rBV	1254972	1236435	35.61%	3.477%
12	10.557	1435	1440	1451	rBV	2205618	2136891	61.54%	6.010%
13	11.251	1554	1558	1561	rBV	1235487	1200348	34.57%	3.376%
14	11.786	1646	1649	1659	rBV2	580266	677980	19.53%	1.907%
15	12.457	1759	1763	1766	rBV	176015	160575	4.62%	0.452%
16	12.568	1779	1782	1796	rBV	197297	267959	7.72%	0.754%
17	12.680	1796	1801	1806	rBV	157084	178655	5.15%	0.502%
18	12.833	1822	1827	1830	rBV	3338377	3209483	92.43%	9.026%
19	13.051	1861	1864	1866	rBV2	34349	37157	1.07%	0.104%
20	13.115	1871	1875	1880	rBV2	28580	38891	1.12%	0.109%
21	13.415	1919	1926	1929	rBV4	32285	54583	1.57%	0.154%
22	13.521	1940	1944	1948	rVB3	38571	59399	1.71%	0.167%
23	13.733	1976	1980	1989	rBV	704410	816923	23.53%	2.297%
24	13.874	1999	2004	2007	rBV	1492377	1506217	43.38%	4.236%
25	13.957	2015	2018	2021	rBV5	38204	56989	1.64%	0.160%
26	14.057	2032	2035	2038	rBV2	82656	84048	2.42%	0.236%
27	14.368	2084	2088	2094	rBV	379749	506279	14.58%	1.424%
28	14.656	2134	2137	2144	rBV	109024	114349	3.29%	0.322%
29	14.792	2156	2160	2164	rVB	283510	284774	8.20%	0.801%
30	14.886	2173	2176	2179	rBV	64648	93291	2.69%	0.262%
31	14.974	2188	2191	2193	rBV	236117	261910	7.54%	0.737%
32	14.998	2193	2195	2202	rVB	318590	392318	11.30%	1.103%
33	15.286	2239	2244	2249	rBV	725514	871930	25.11%	2.452%
34	15.333	2249	2252	2258	rVB	113697	142804	4.11%	0.402%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.515	2280	2283	2288	rVB	80774	106427	3.07%	0.299%
36	15.745	2317	2322	2326	rBV	252134	362802	10.45%	1.020%
37	15.792	2326	2330	2337	rVV	134111	251757	7.25%	0.708%
38	16.768	2492	2496	2502	rVB3	81462	140644	4.05%	0.396%

Sum of corrected areas: 35557335

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
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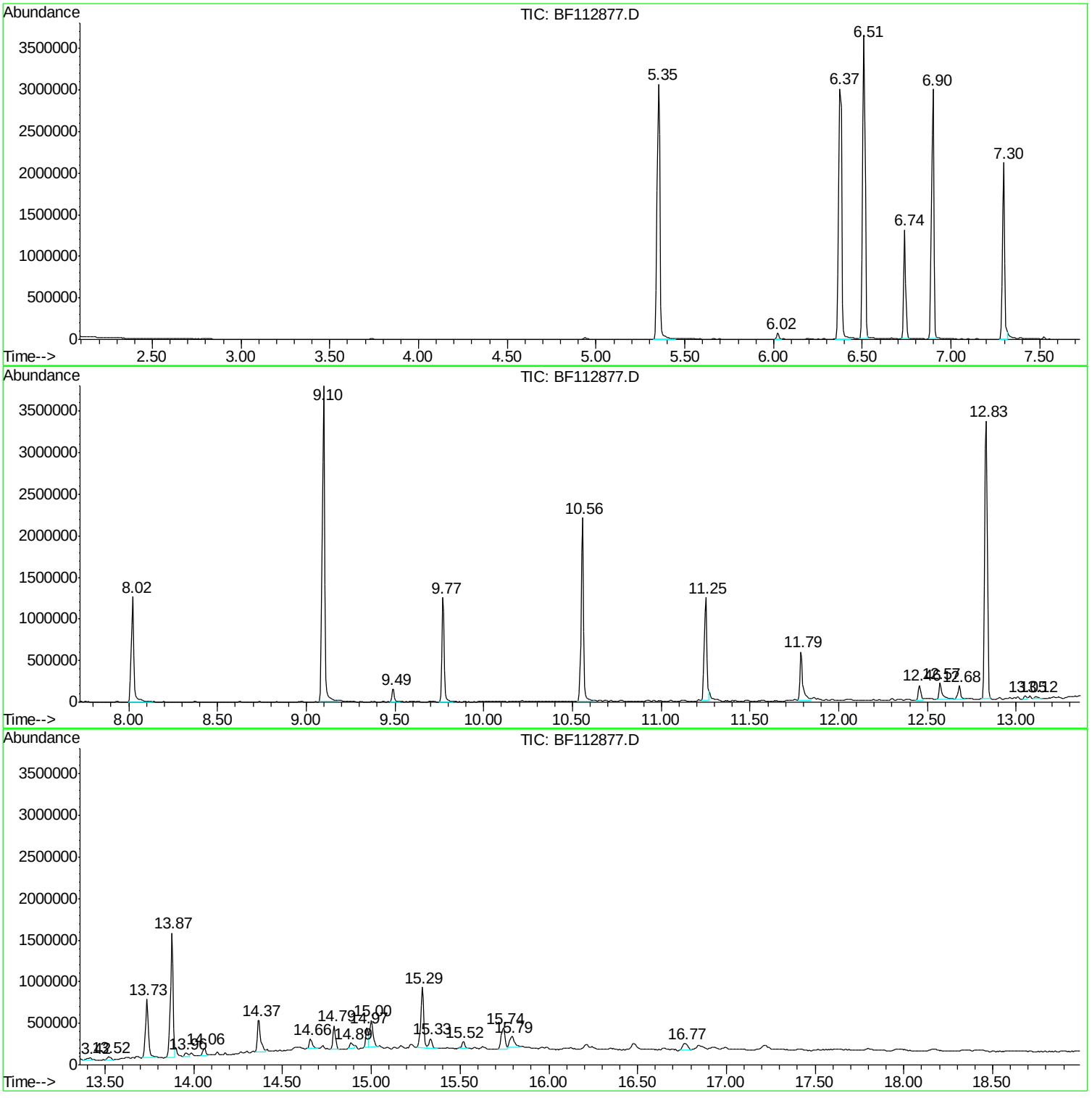
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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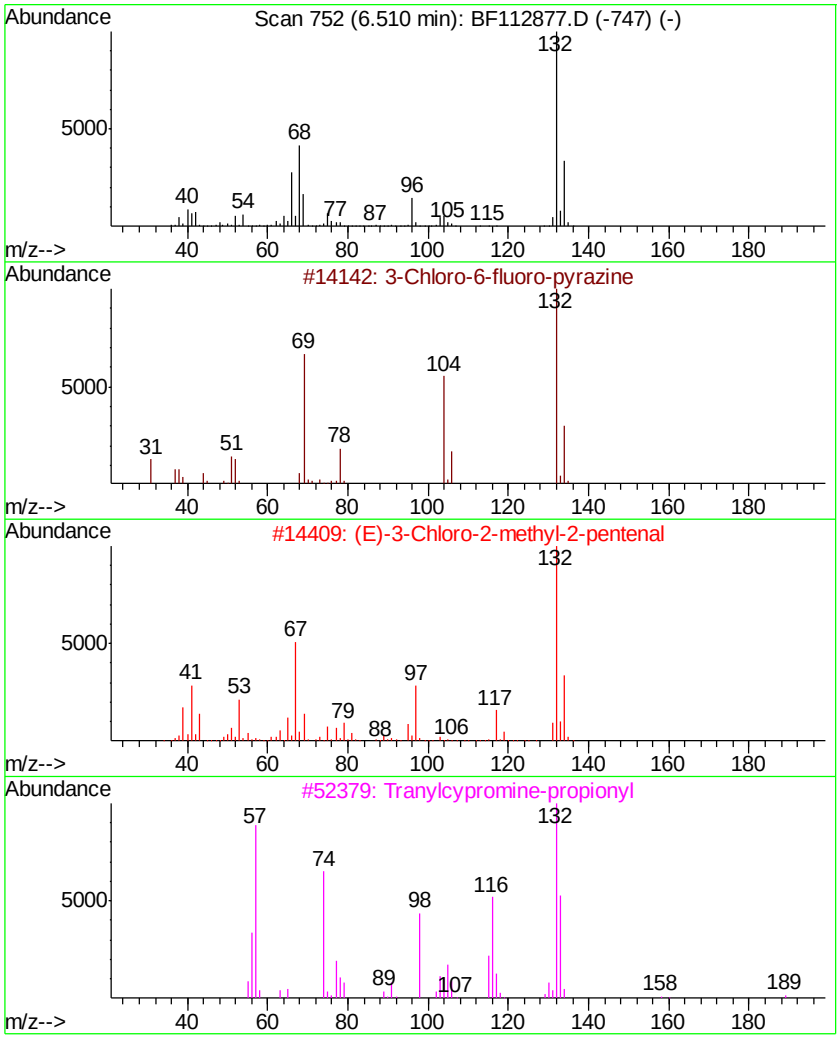
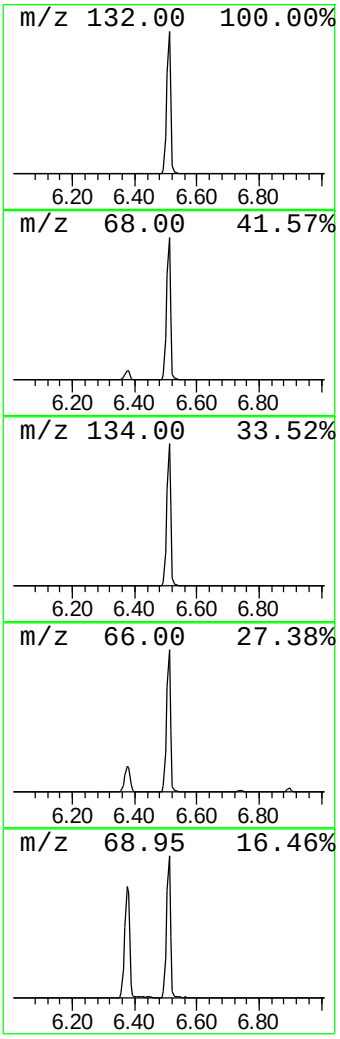
Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	64.35 ng	3324200	1,4-Dichlorobenzene-d4	6.74

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF112877.D
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Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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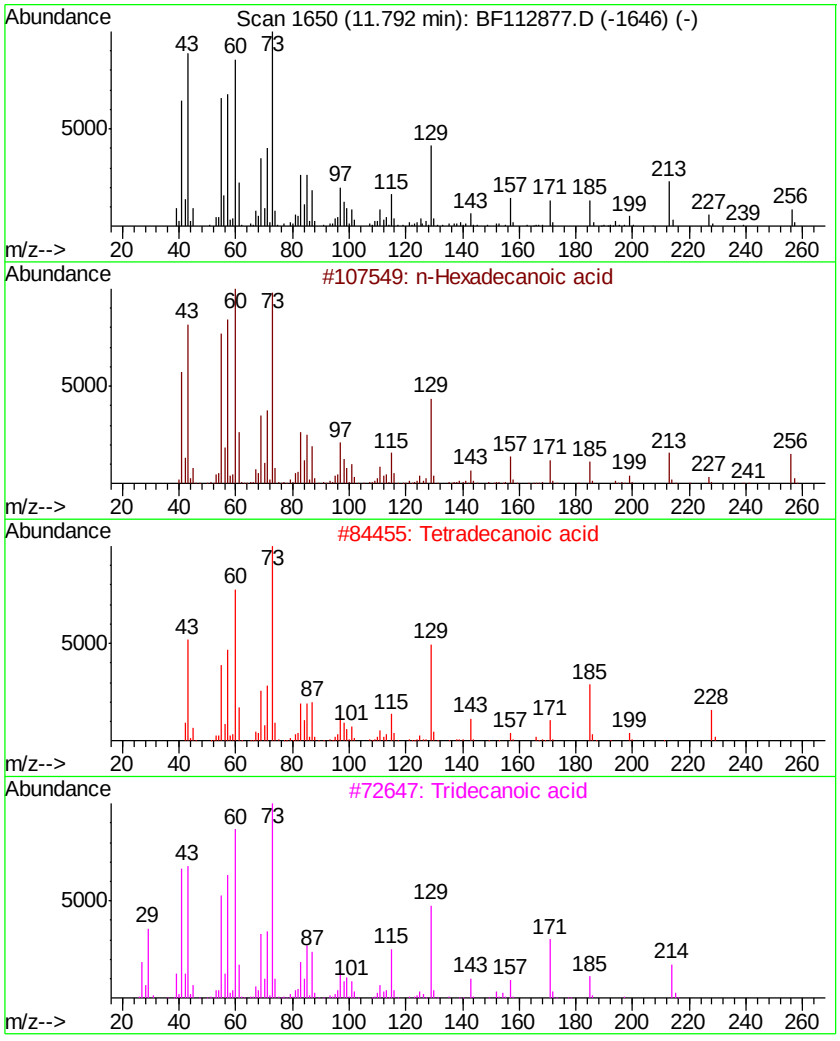
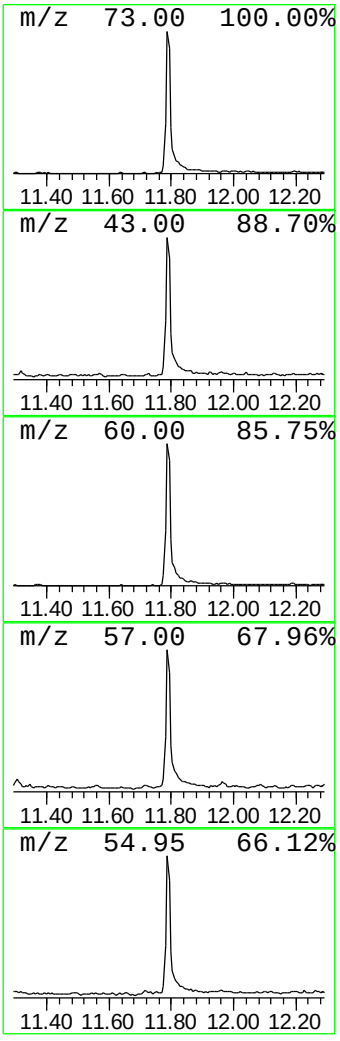
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	11.30 ng	677980	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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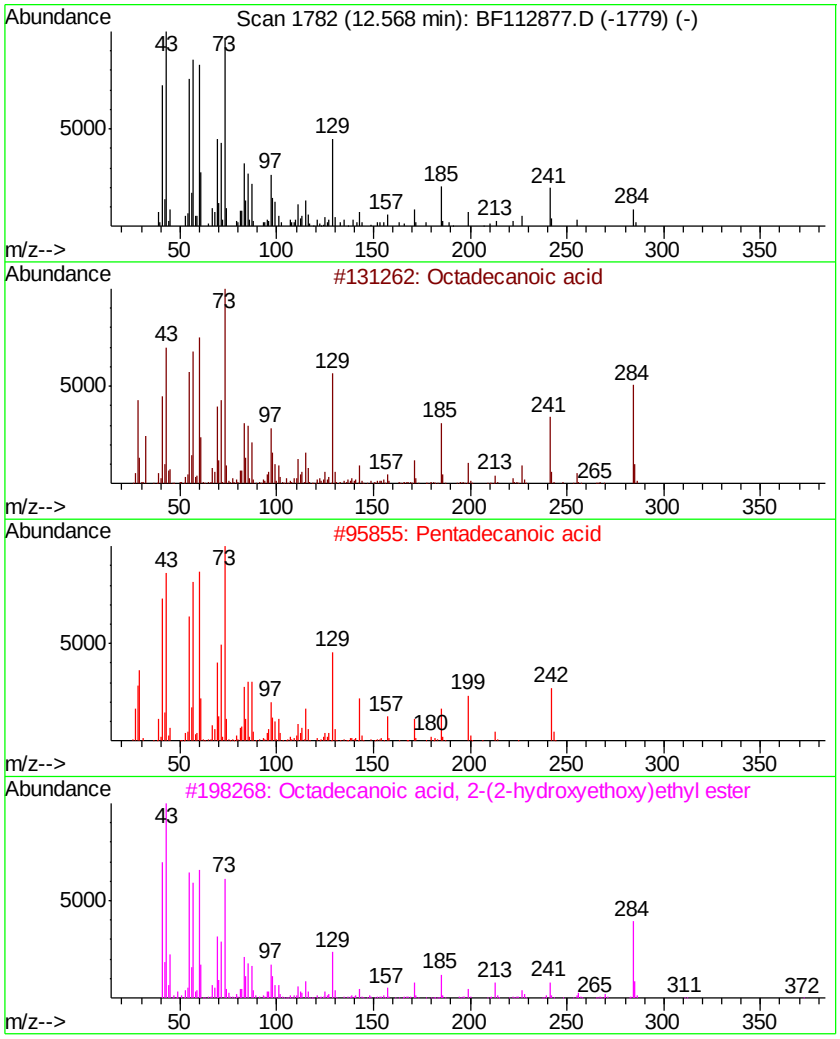
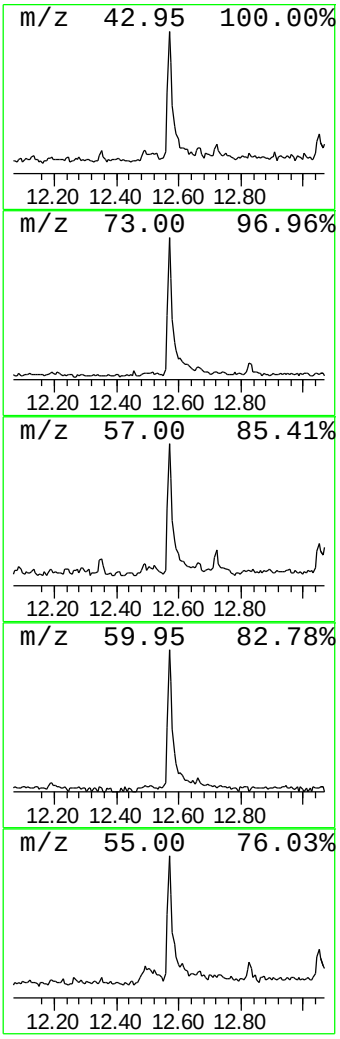
Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.56 ng	267959	Chrysene-d12	13.87

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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

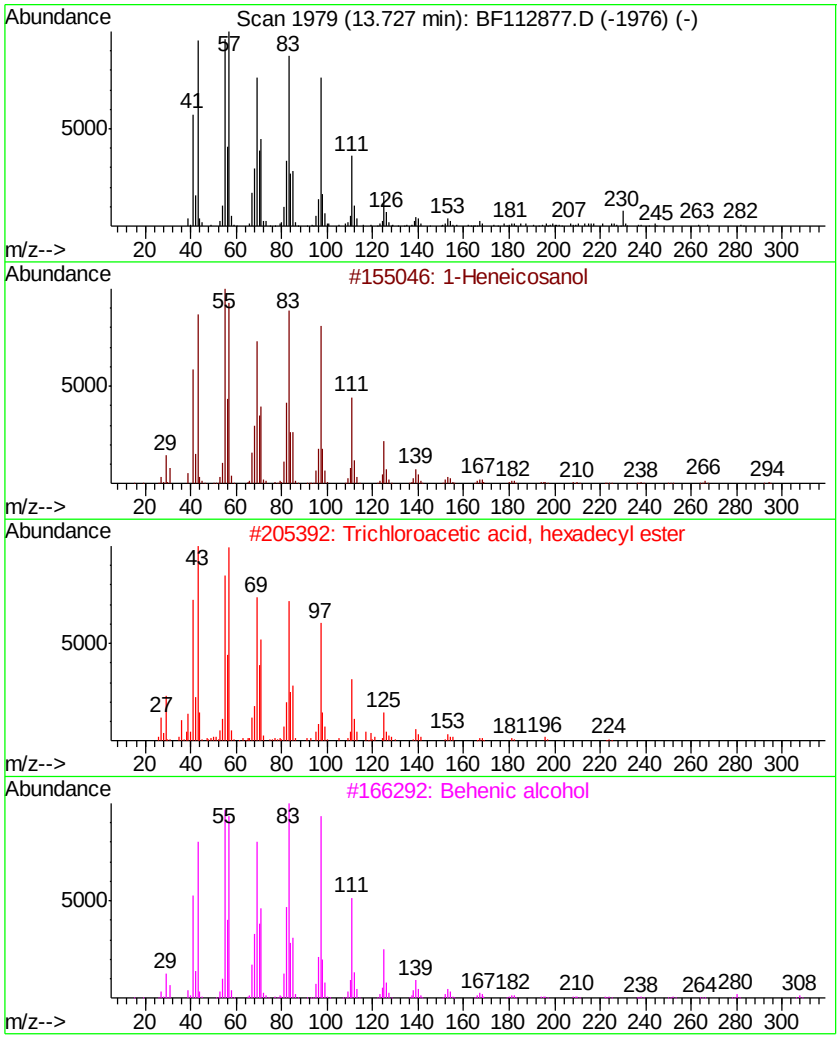
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

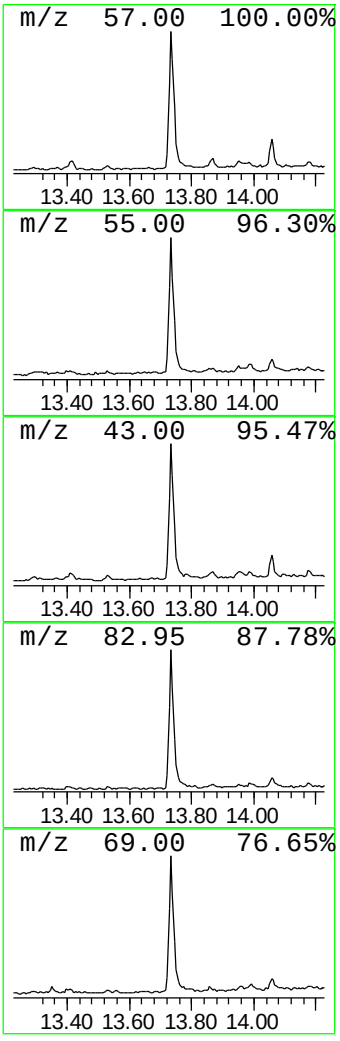
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	10.85 ng	816923	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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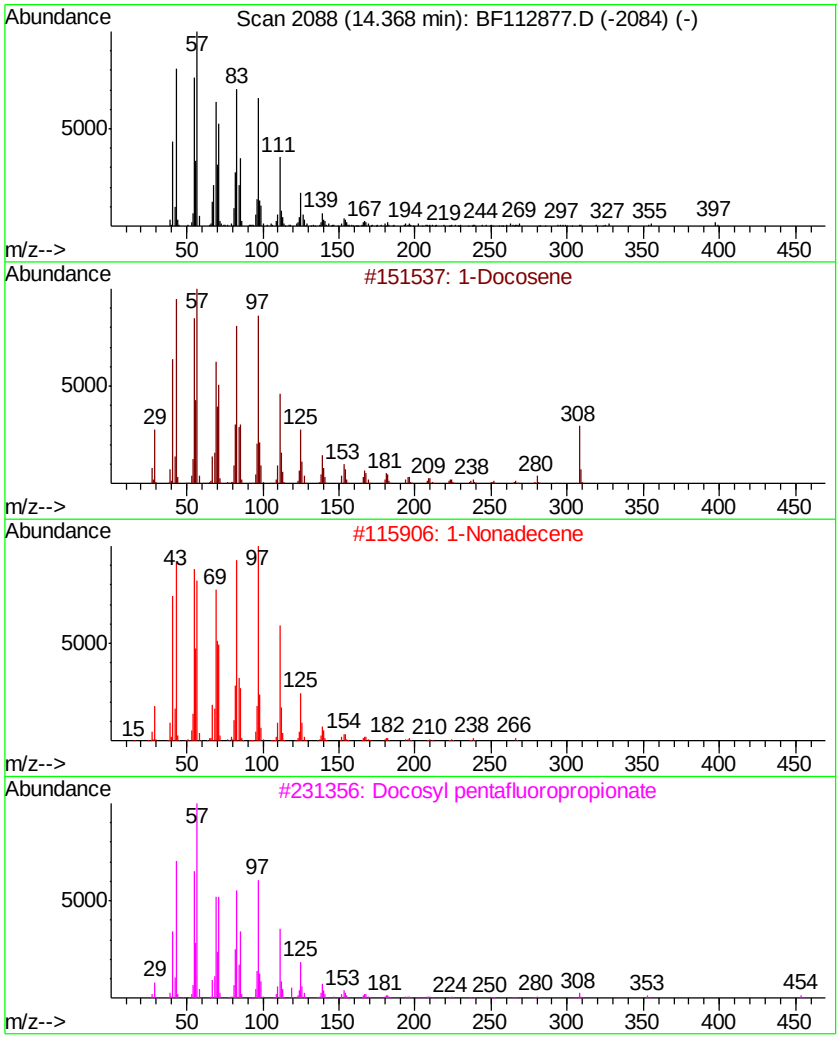
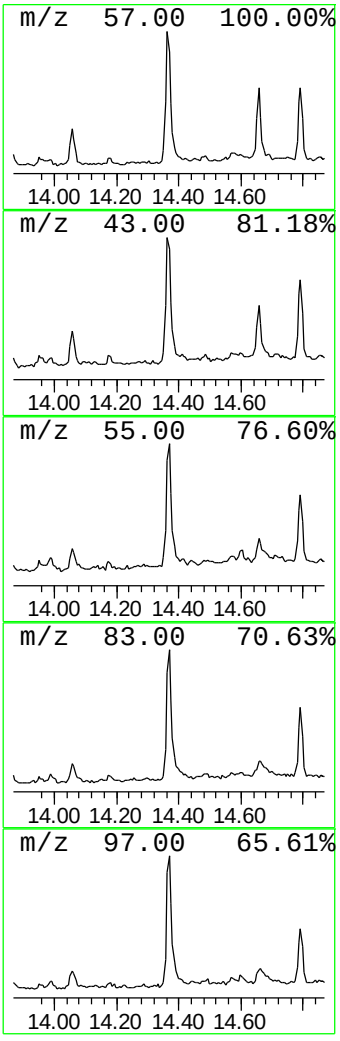
Peak Number 7 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	6.72 ng	506279	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	1-Nonadecene	266	C19H38	018435-45-5	97
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





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Sample : K1705-15
Misc :
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Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

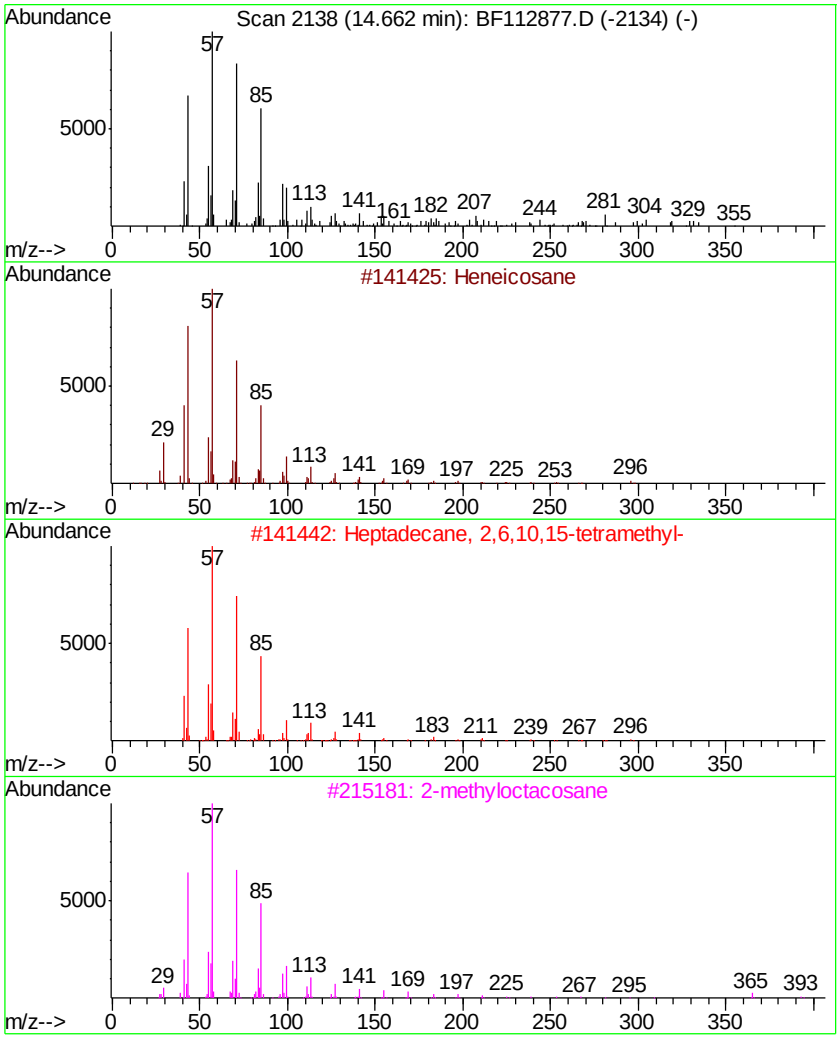
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

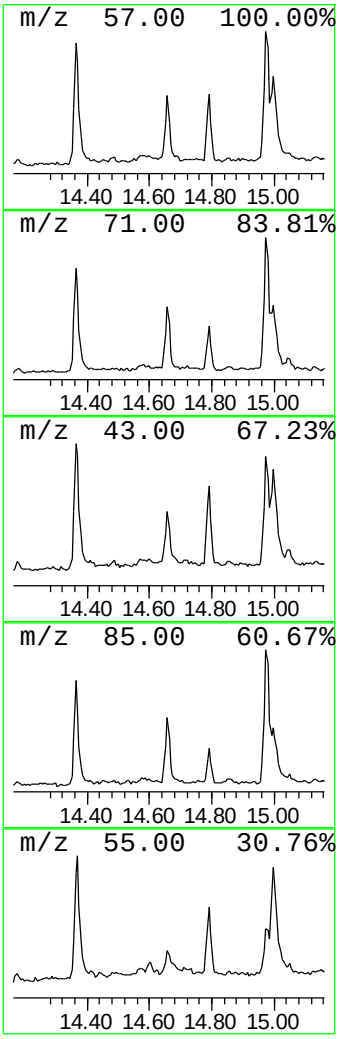
****

Peak Number 8 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.62 ng	114349	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Nonadecane	268	C19H40	000629-92-5	80





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Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

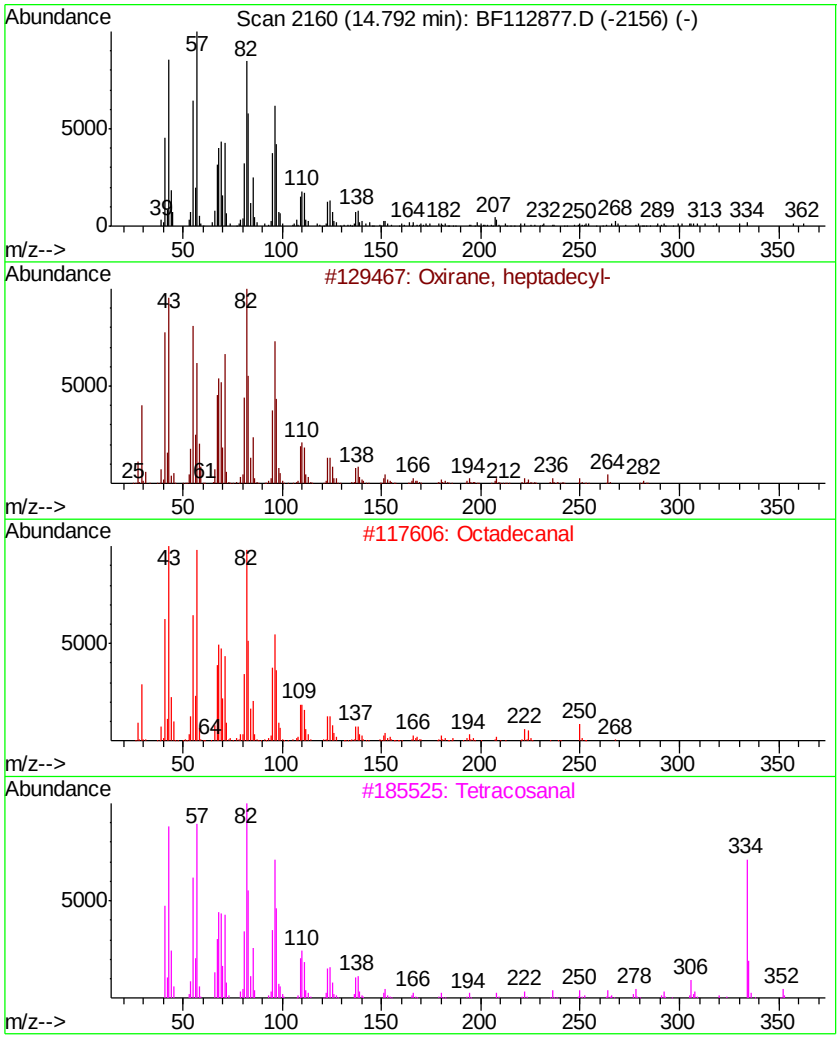
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

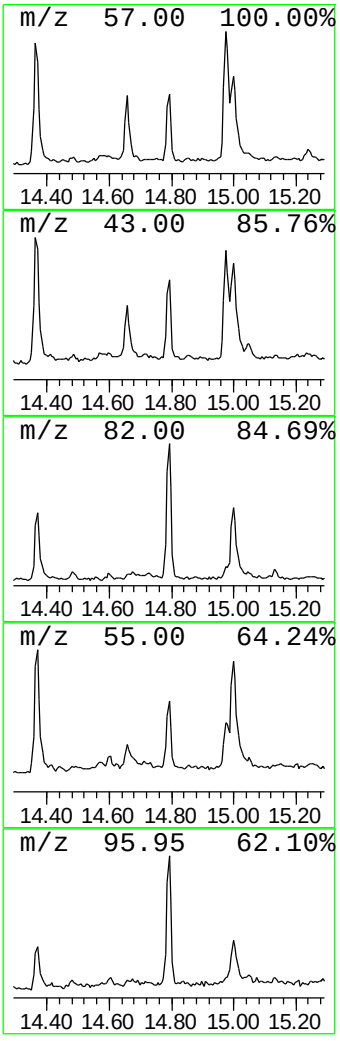
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	6.53 ng	284774	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Tetracosanal	352	C24H48O	057866-08-7	91
4	Tetradecanal	212	C14H28O	000124-25-4	91
5	12-Octadecenal	266	C18H34O	056554-91-7	90





Library Search Compound Report

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Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
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Sample : K1705-15
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Instrument :
BNA_F
ClientSampleId :
PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

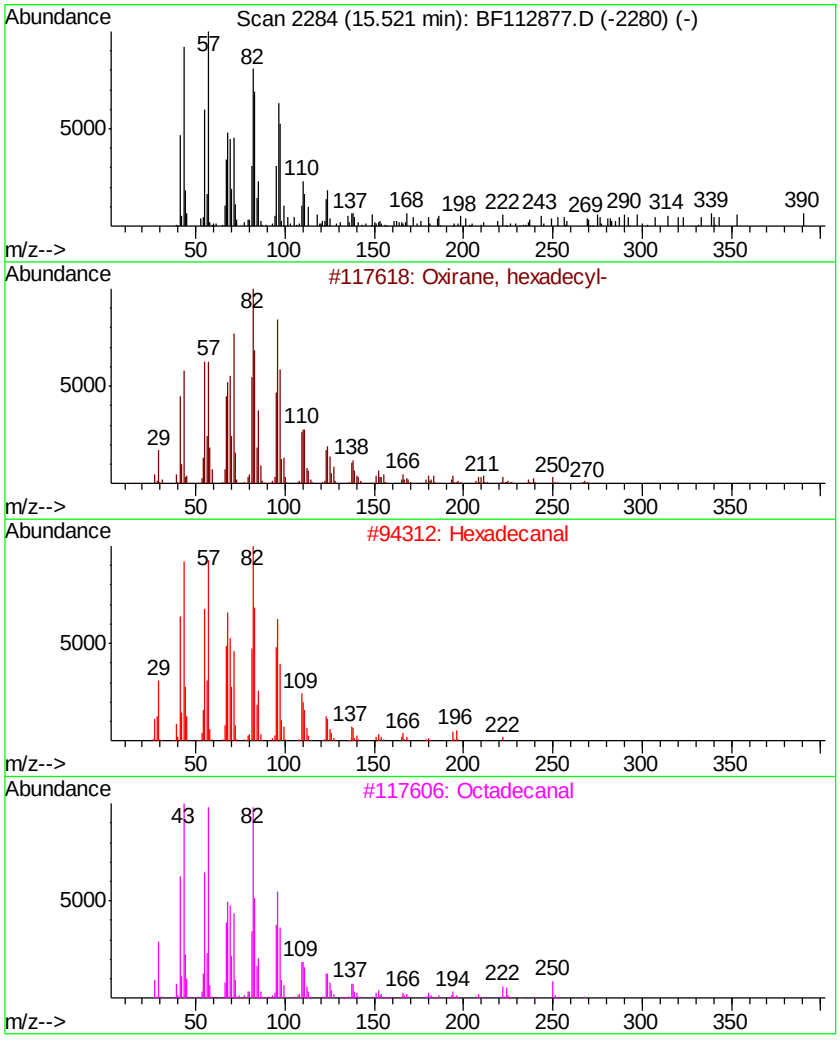
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

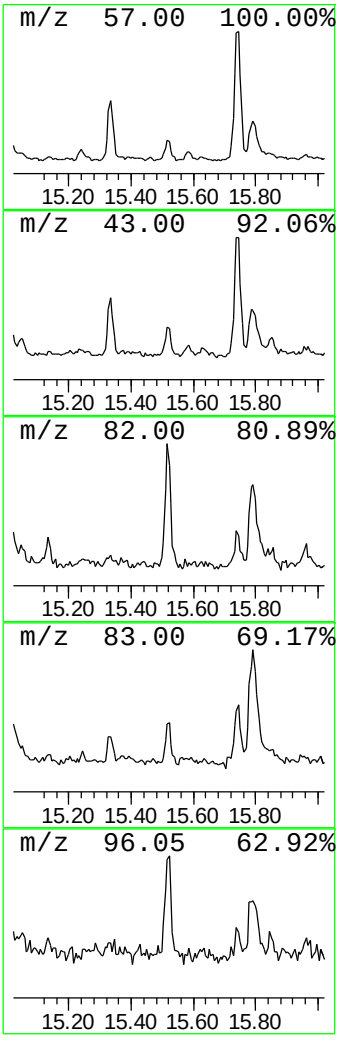
****

Peak Number 13 Oxirane, hexadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.52	2.44 ng	106427	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Hexadecanal	240	C16H32O	000629-80-1	91
3	Octadecanal	268	C18H36O	000638-66-4	90
4	14-Octadecenal	266	C18H34O	056554-89-3	80
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	68





Library Search Compound Report

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Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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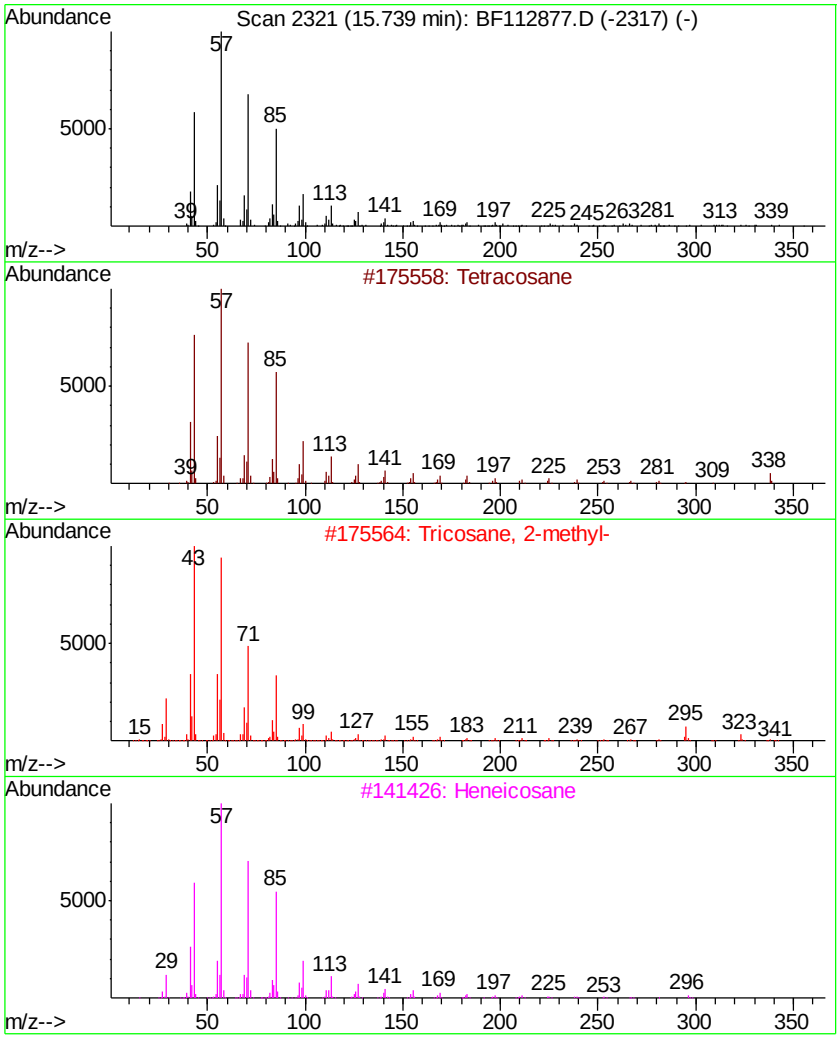
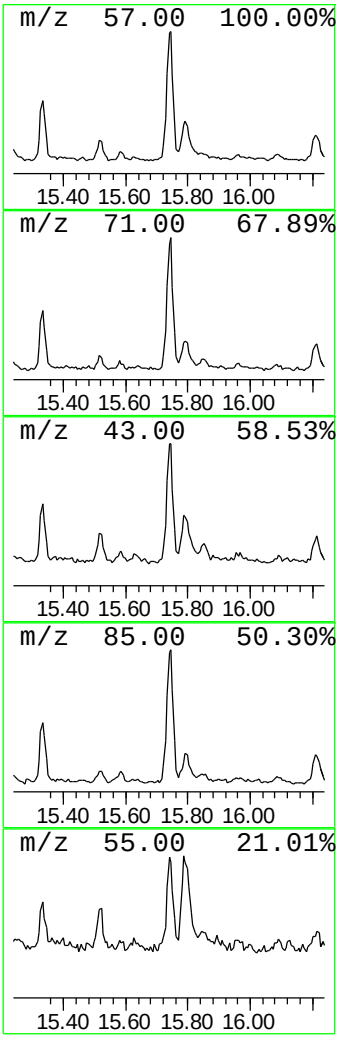
Peak Number 14 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	8.32 ng	362802	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

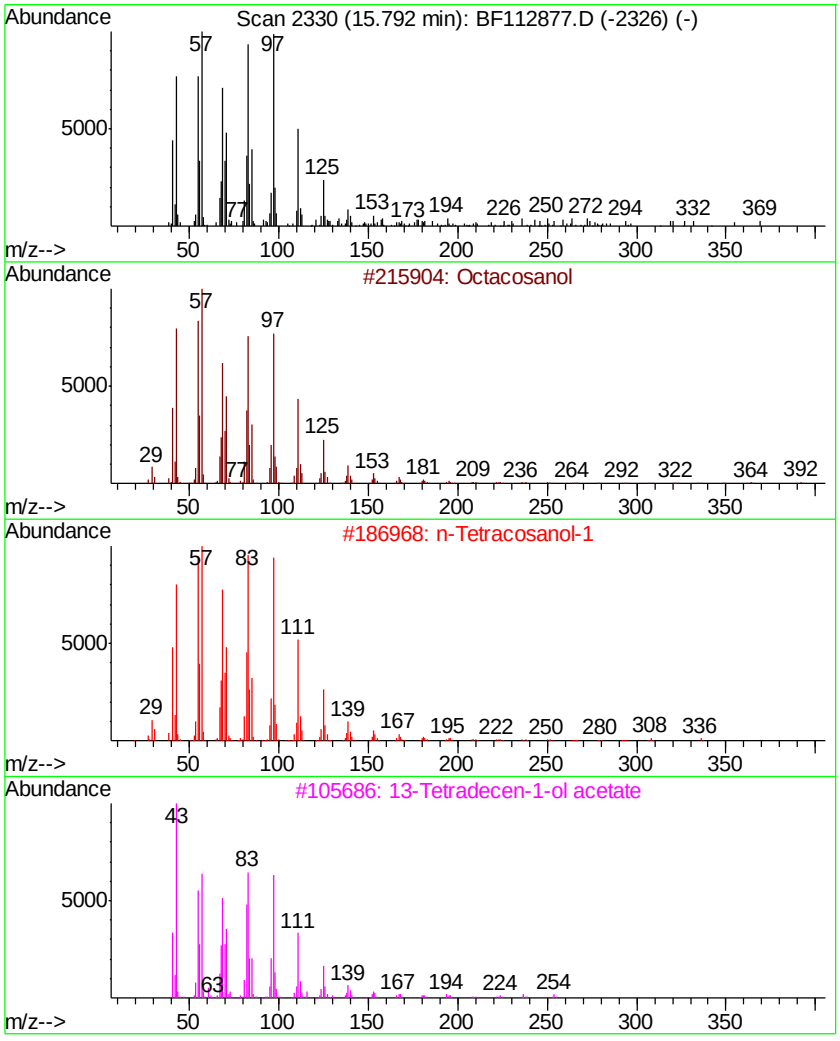
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

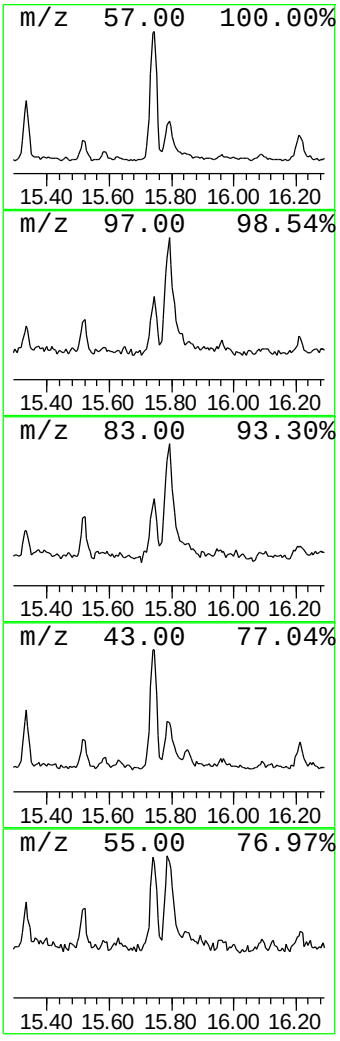
****

Peak Number 15 Octacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	5.77 ng	251757	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
4	Cycloeicosane	280	C20H40	000296-56-0	91
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112877.D
Acq On : 6 Mar 2019 2:56
Operator : JU/SJ
Sample : K1705-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-028-B097-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.51	6.51	64.3	ng	3324200	1	6.74	1033150	20.0
n-Hexadecanoic acid	11.79	11.3	ng	677980	4	11.25	1200350	20.0
Octadecanoic acid	12.57	3.6	ng	267959	5	13.87	1506220	20.0
1-Heneicosanol	13.73	10.9	ng	816923	5	13.87	1506220	20.0
1-Docosene	14.37	6.7	ng	506279	5	13.87	1506220	20.0
Heneicosane	14.66	2.6	ng	114349	6	15.29	871930	20.0
Oxirane, heptadecyl-	14.79	6.5	ng	284774	6	15.29	871930	20.0
Oxirane, hexadecyl-	15.52	2.4	ng	106427	6	15.29	871930	20.0
Tetracosane	15.74	8.3	ng	362802	6	15.29	871930	20.0
Octacosanol	15.79	5.8	ng	251757	6	15.29	871930	20.0