LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

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-BF040820.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	5.269	537	541	552	rBV	3314339	3046656	85.90%	10.468%
2	6.316	714	719	735	rBV	2932350	3039040	85.69%	10.442%
3	6.663	774	778	782	rBV	1225411	967089	27.27%	3.323%
4	6.822	800	805	808	rBV	3022135	2588733	72.99%	8.895%
5	7.234	870	875	878	rBV	2226052	2022225	57.02%	6.948%
6	7.951	993	997	1000	rBV	1347552	1219483	34.38%	4.190%
7	9.027	1175	1180	1183	rBV	4287520	3546578	100.00%	12.186%
8	9.422	1244	1247	1251	rBV	501877	381411	10.75%	1.310%
9	9.698	1291	1294	1298	rBV	1396263	1220435	34.41%	4.193%
10	10.492	1424	1429	1432	rBV	1778231	1686762	47.56%	5.795%
11	11.186	1543	1547	1549	rBV	1129407	1071837	30.22%	3.683%
12	11.204	1549	1550	1554	rVV	438142	310192	8.75%	1.066%
13	11.257	1554	1559	1563	rVB	112124	97074	2.74%	0.334%
14	11.686	1628	1632	1634	rBV	57477	53404	1.51%	0.183%
15	11.721	1634	1638	1642	rBV2	212617	260984	7.36%	0.897%
16	11.792	1647	1650	1653	rBV2	71950	80173	2.26%	0.275%
17	11.980	1679	1682	1684	rBV2	50416	45651	1.29%	0.157%
18	12.316	1736	1739	1743	rBV	42269	42237	1.19%	0.145%
19	12.392	1748	1752	1756	rBV	568273	451144	12.72%	1.550%
20	12.445	1758	1761	1765	rVB2	44475	49402	1.39%	0.170%
21	12.510	1769	1772	1776	rBV3	58036	68492	1.93%	0.235%
22	12.621	1785	1791	1794	rBV2	409326	473053	13.34%	1.625%
23	12.674	1797	1800	1804	rVB3	35861	41061	1.16%	0.141%
24	12.768	1812	1816	1820	rVB	2625181	2454761	69.21%	8.434%
25	12.845	1823	1829	1831	rBV3	40559	66925	1.89%	0.230%
26	12.951	1844	1847	1850	rVB	57767	64186	1.81%	0.221%
27	13.051	1861	1864	1868	rBV2	63201	66745	1.88%	0.229%
28	13.257	1894	1899	1905	rBV	259296	239692	6.76%	0.824%
29	13.457	1930	1933	1937	rVB	51445	56377	1.59%	0.194%
30	13.674	1966	1970	1980	rBV2	195770	342599	9.66%	1.177%
31	13.815	1989	1994	1997	rBV2	960433	1099290	31.00%	3.777%
32	13.845	1997	1999	2001	rVB	174913	145091	4.09%	0.499%
33	14.204	2058	2060	2064	rVB	52212	41613	1.17%	0.143%
34	14.298	2074	2076	2079	rBV	53933	51954	1.46%	0.179%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

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-BF040820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.598	2125	2127	2132	rVB	70375	75620	2.13%	0.260%
36	14.827	2162	2166	2169	rBV	195774	279715	7.89%	0.961%
37	14.904	2177	2179	2186	rVB3	85795	140509	3.96%	0.483%
38	15.104	2211	2213	2219	rVB	102956	115528	3.26%	0.397%
39	15.162	2220	2223	2228	rBV	159565	194347	5.48%	0.668%
40	15.221	2229	2233	2237	rBV	582523	697149	19.66%	2.395%
41	17.903	2688	2689	2696	rVB7	35312	59394	1.67%	0.204%
42	18.027	2706	2710	2713	rBV5	36539	65731	1.85%	0.226%
43	18.256	2747	2749	2752	rBV4	28459	42534	1.20%	0.146%
44	18.933	2862	2864	2869	rBV5	21658	41855	1.18%	0.144%

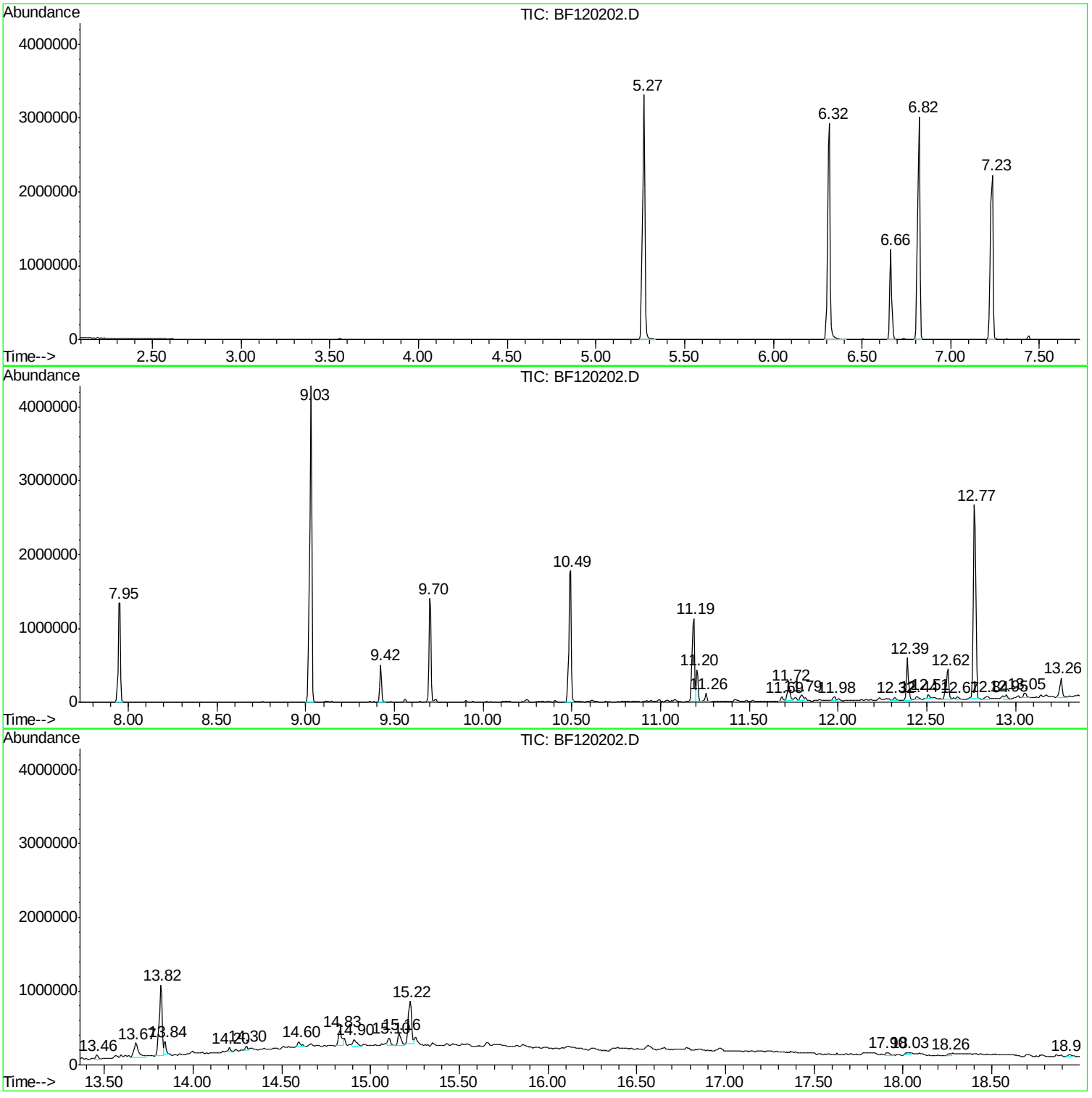
Sum of corrected areas: 29104731

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

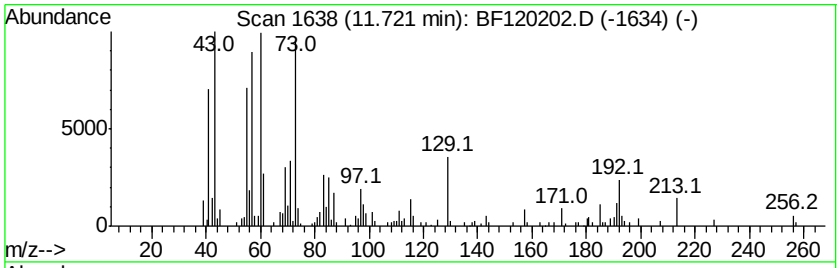
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

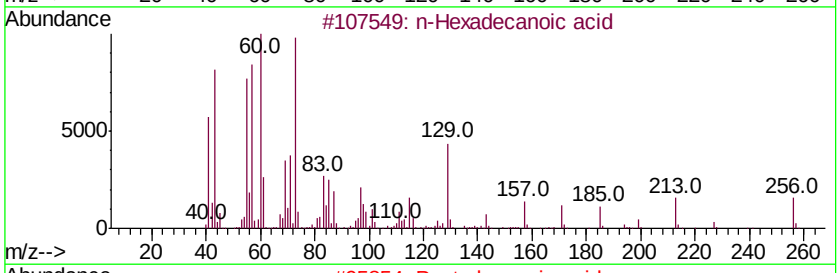
****

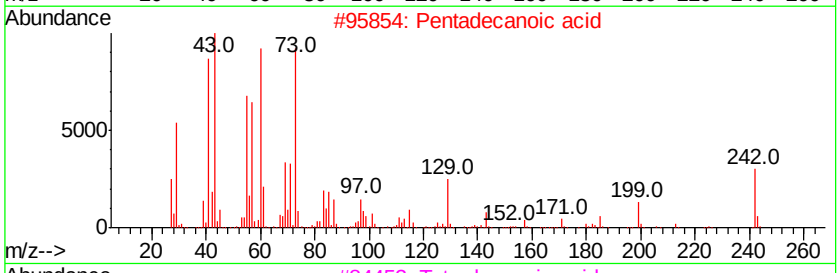
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

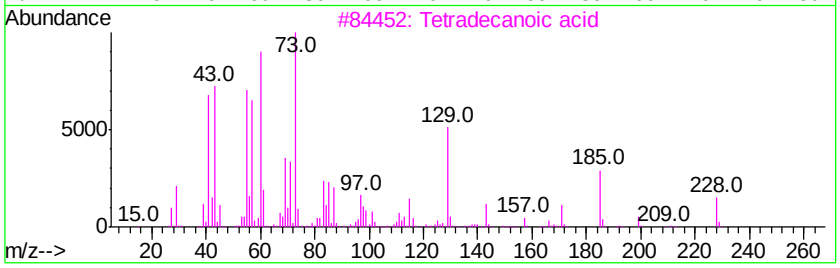
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	4.87 ng	260984	Phenanthrene-d10	11.19

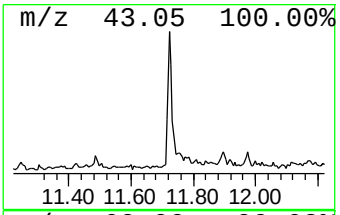
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53

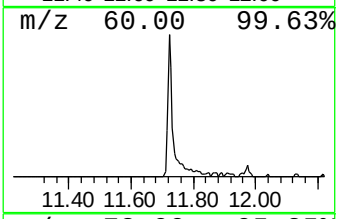


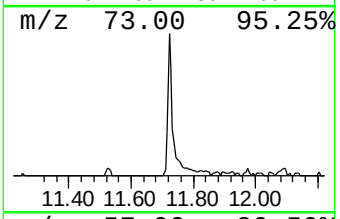


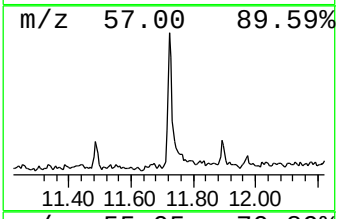


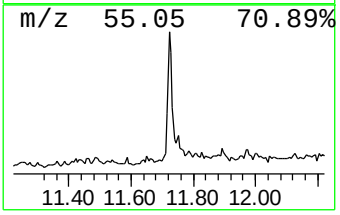












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

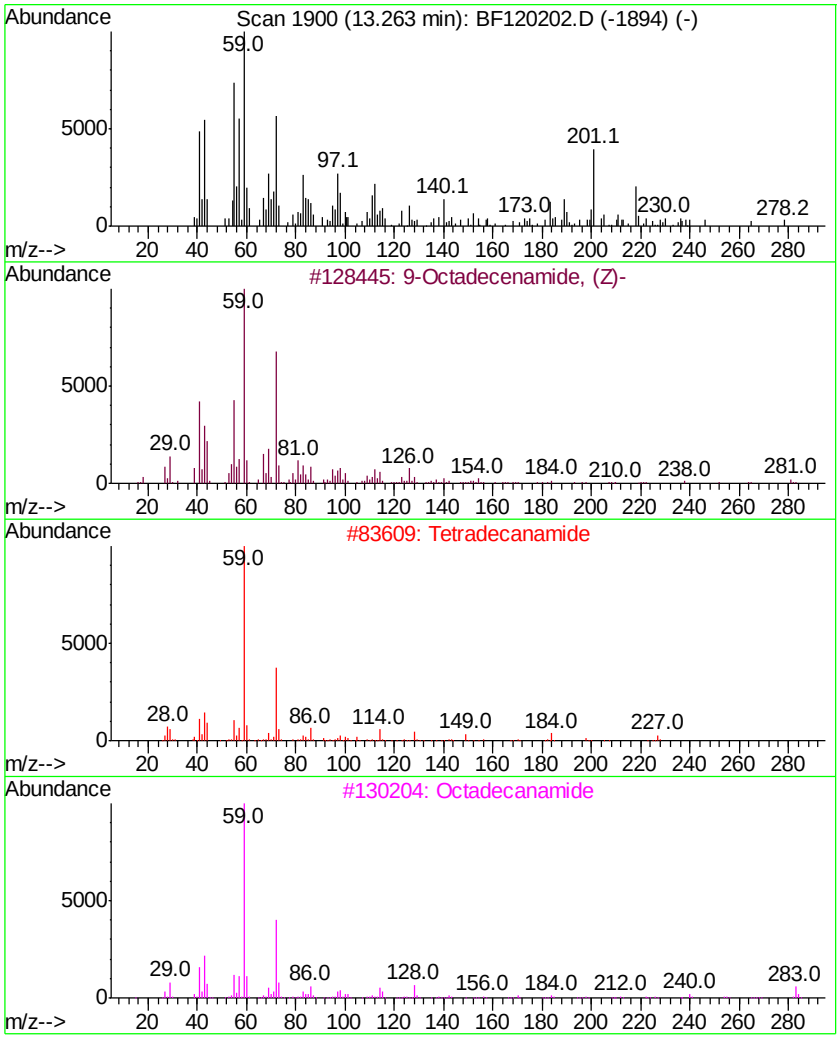
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

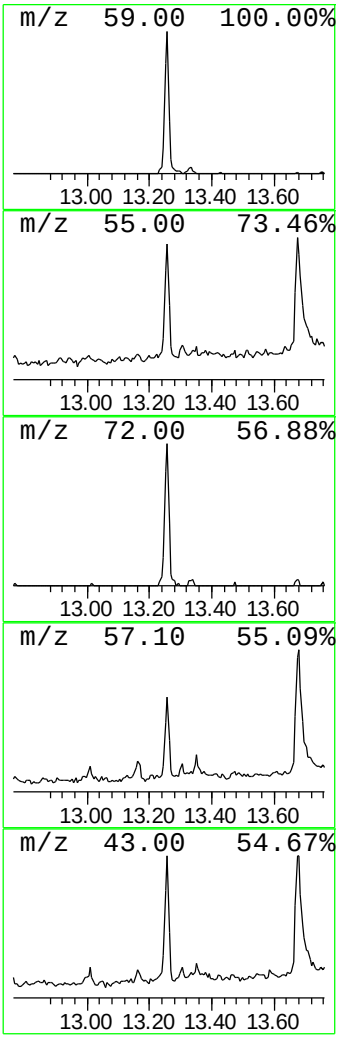
****

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	4.36 ng	239692	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	52
2	Tetradecanamide	227	C14H29NO	000638-58-4	50
3	Octadecanamide	283	C18H37NO	000124-26-5	50
4	7-Nonenamide	155	C9H17NO	090949-53-4	47
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	46





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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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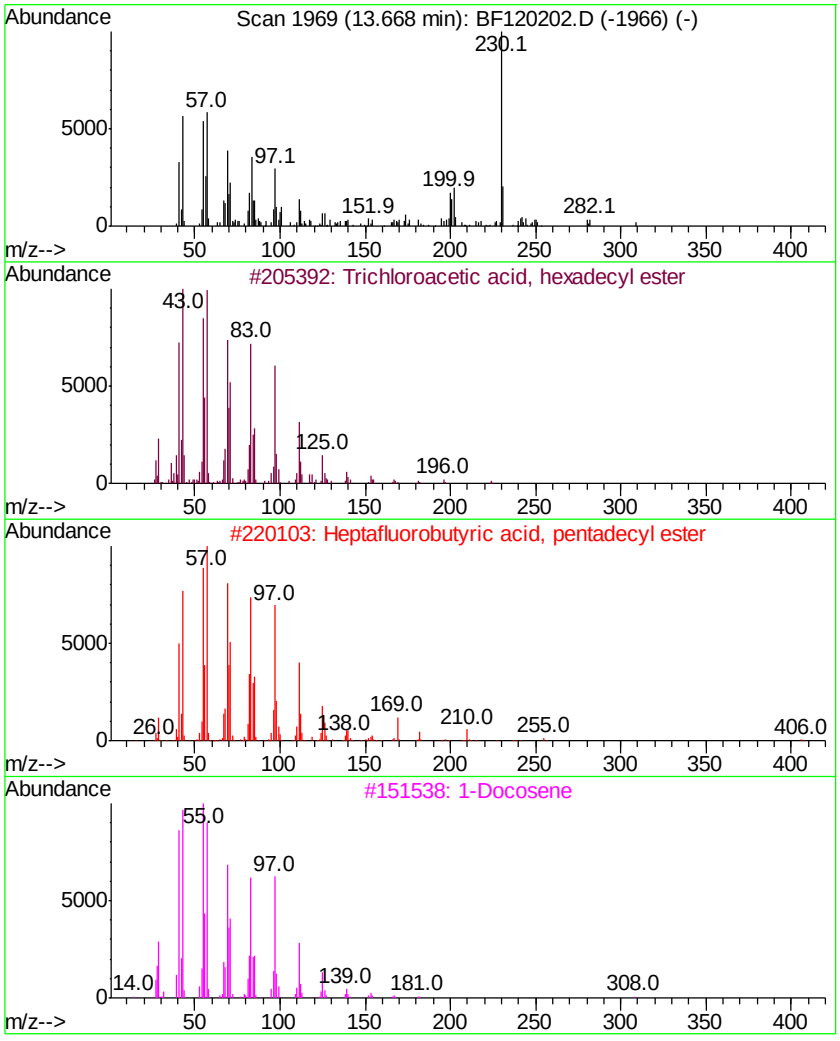
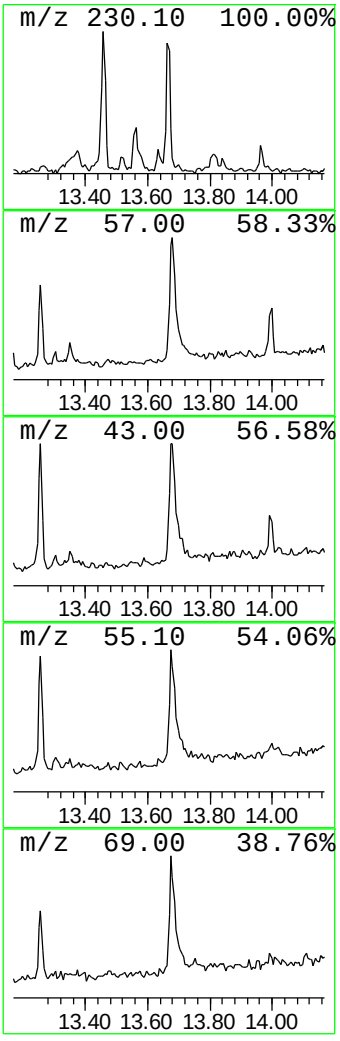
Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	6.23 ng	342599	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	1-Docosene	308	C22H44	001599-67-3	93
4	Cyclotetradecane	196	C14H28	000295-17-0	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

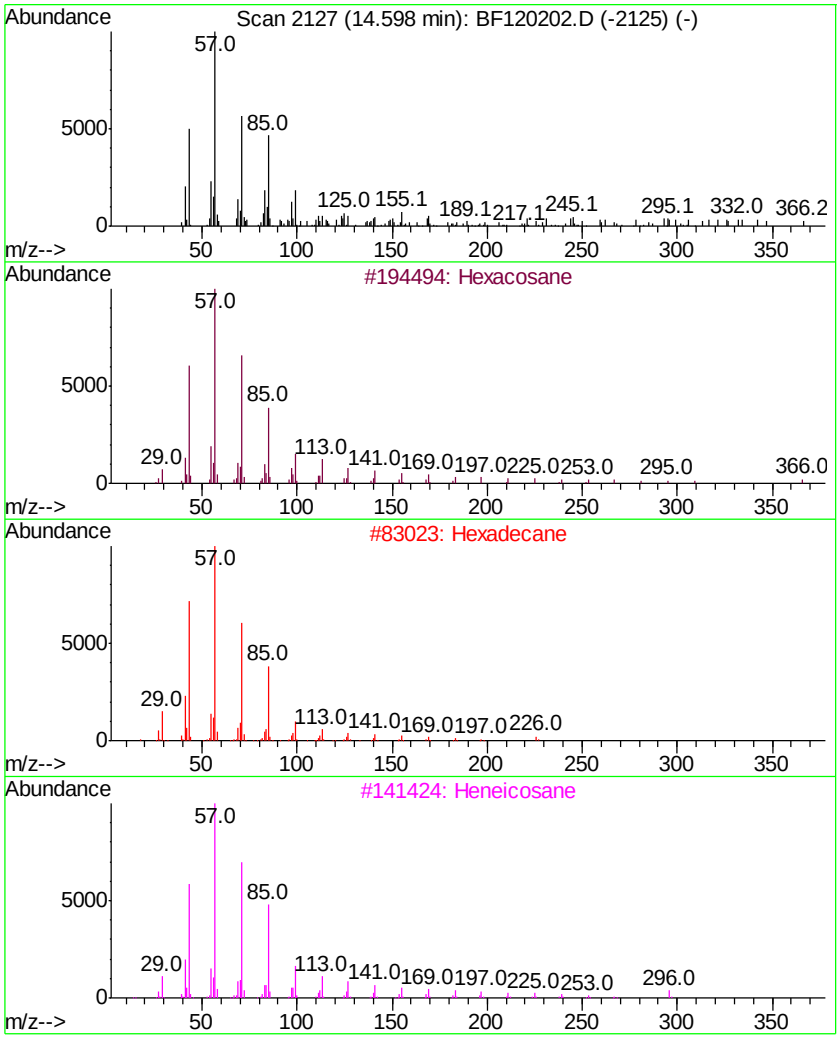
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

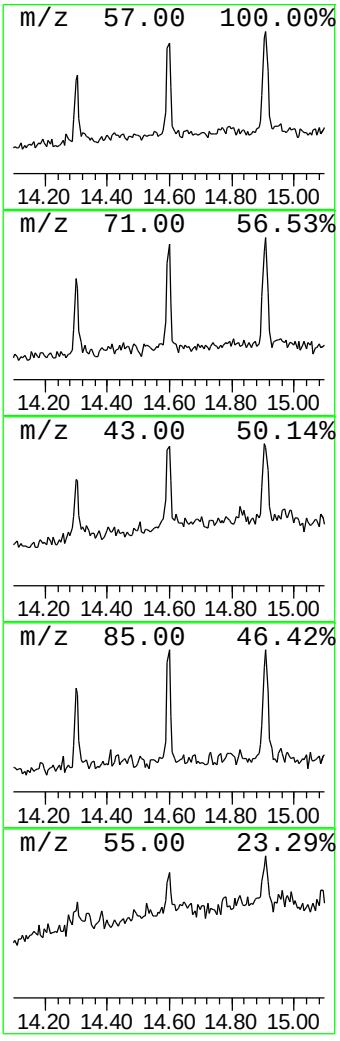
****

Peak Number 5 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.17 ng	75620	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	89
2	Hexadecane	226	C16H34	000544-76-3	70
3	Heneicosane	296	C21H44	000629-94-7	70
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	70
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

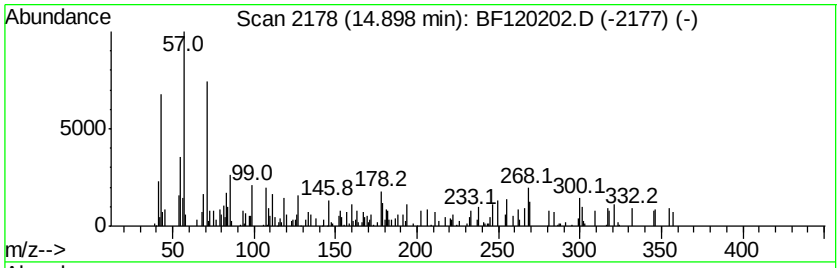
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

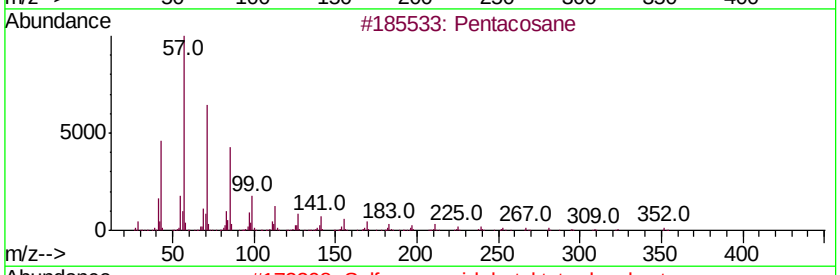
****

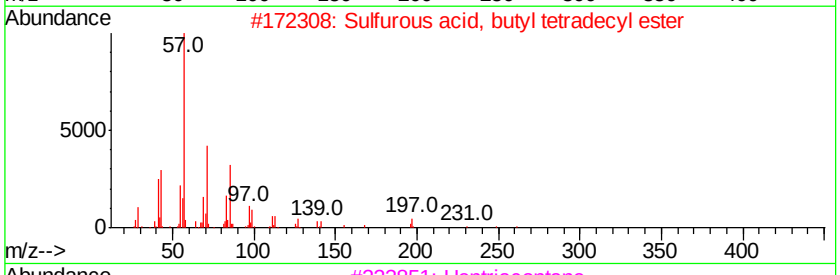
Peak Number 6 Pentacosane Concentration Rank 5

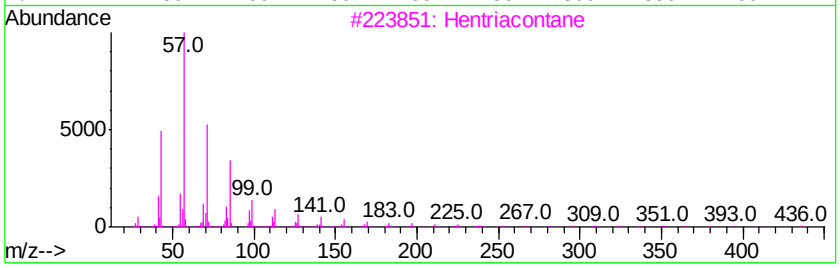
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	4.03 ng	140509	Perylene-d12	15.22

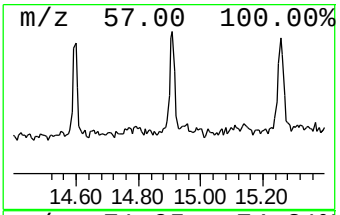
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
3	Hentriacontane	437	C31H64	000630-04-6	80
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
5	Hexatriacontane	507	C36H74	000630-06-8	80

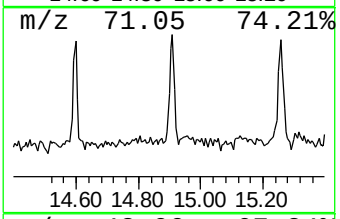


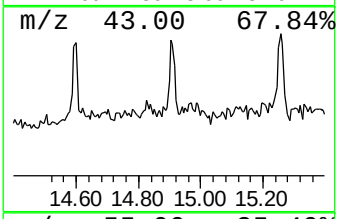


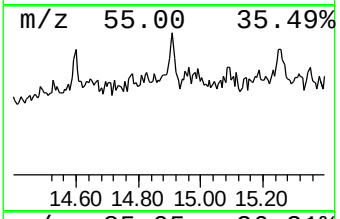


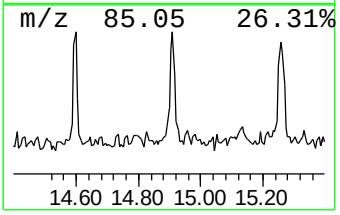












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042420\
Data File : BF120202.D
Acq On : 24 Apr 2020 15:12
Operator : MA/SJ
Sample : L2378-07
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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
n-Hexadecanoic acid	11.72	4.9	ng	260984	4	11.19	1071840	20.0
9-Octadecenamide,...	13.26	4.4	ng	239692	5	13.82	1099290	20.0
Trichloroacetic a...	13.67	6.2	ng	342599	5	13.82	1099290	20.0
Hexacosane	14.60	2.2	ng	75620	6	15.22	697149	20.0
Pentacosane	14.90	4.0	ng	140509	6	15.22	697149	20.0