LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	483	486	501	rBV	17570	31810	1.29%	0.161%
2	5.346	551	554	578	rBV	1894040	2251363	91.22%	11.361%
3	6.375	726	729	754	rBV	2198980	2290088	92.79%	11.557%
4	6.581	762	764	782	rBV	23117	63722	2.58%	0.322%
5	6.722	785	788	798	rVB	667157	568793	23.05%	2.870%
6	7.293	881	885	909	rBV	1565663	1592256	64.51%	8.035%
7	8.010	1003	1007	1021	rBV	721867	712058	28.85%	3.593%
8	9.081	1185	1189	1200	rBV	2748171	2468133	100.00%	12.455%
9	9.481	1254	1257	1263	rBV	345130	290318	11.76%	1.465%
10	9.757	1300	1304	1308	rBV	785010	716750	29.04%	3.617%
11	10.551	1436	1439	1455	rBV	1150720	1106006	44.81%	5.581%
12	11.245	1554	1557	1560	rBV	693363	633005	25.65%	3.194%
13	11.269	1560	1561	1565	rVB	123148	87947	3.56%	0.444%
14	11.780	1645	1648	1651	rBV2	39929	47079	1.91%	0.238%
15	12.463	1761	1764	1769	rBV	275988	239777	9.71%	1.210%
16	12.563	1778	1781	1788	rBV	80994	103640	4.20%	0.523%
17	12.692	1797	1803	1807	rBV	223324	231600	9.38%	1.169%
18	12.833	1822	1827	1830	rBV	2150074	2018635	81.79%	10.187%
19	13.057	1862	1865	1868	rBV	46636	46548	1.89%	0.235%
20	13.304	1903	1907	1911	rBV2	58388	60362	2.45%	0.305%
21	13.398	1919	1923	1925	rBV2	26897	29792	1.21%	0.150%
22	13.539	1944	1947	1954	rVB	31225	34103	1.38%	0.172%
23	13.751	1975	1983	1997	rVB7	179894	438996	17.79%	2.215%
24	13.857	1998	2001	2002	rBV	38821	34830	1.41%	0.176%
25	13.892	2002	2007	2010	rVV2	741065	840058	34.04%	4.239%
26	13.916	2010	2011	2019	rVB	135274	104558	4.24%	0.528%
27	14.039	2029	2032	2035	rBV	32054	39720	1.61%	0.200%
28	14.345	2081	2084	2087	rVB	67452	57714	2.34%	0.291%
29	14.386	2087	2091	2101	rBV6	60408	158698	6.43%	0.801%
30	14.504	2108	2111	2116	rVB	188459	156187	6.33%	0.788%
31	14.639	2132	2134	2137	rVB	38919	35039	1.42%	0.177%
32	14.780	2154	2158	2163	rVB2	153216	170236	6.90%	0.859%
33	14.916	2178	2181	2184	rBV	129719	169478	6.87%	0.855%
34	14.963	2187	2189	2192	rVB	103379	92208	3.74%	0.465%
35	15.027	2195	2200	2209	rBV4	105856	277880	11.26%	1.402%
36	15.210	2227	2231	2234	rBV	76865	84833	3.44%	0.428%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.268	2238	2241	2245	rVB	98756	109497	4.44%	0.553%
38	15.327	2246	2251	2259	rBV	608196	752367	30.48%	3.797%
39	15.510	2278	2282	2287	rBV2	76557	98020	3.97%	0.495%
40	15.727	2314	2319	2323	rBV	111302	166758	6.76%	0.842%
41	16.192	2395	2398	2403	rVB2	38370	54949	2.23%	0.277%
42	16.462	2442	2444	2453	rVB4	49860	77975	3.16%	0.393%
43	16.745	2487	2492	2500	rVB2	108133	196633	7.97%	0.992%
44	17.174	2562	2565	2572	rVB	37334	75430	3.06%	0.381%

Sum of corrected areas: 19815849

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
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Acq On : 23 Oct 2020 17:19
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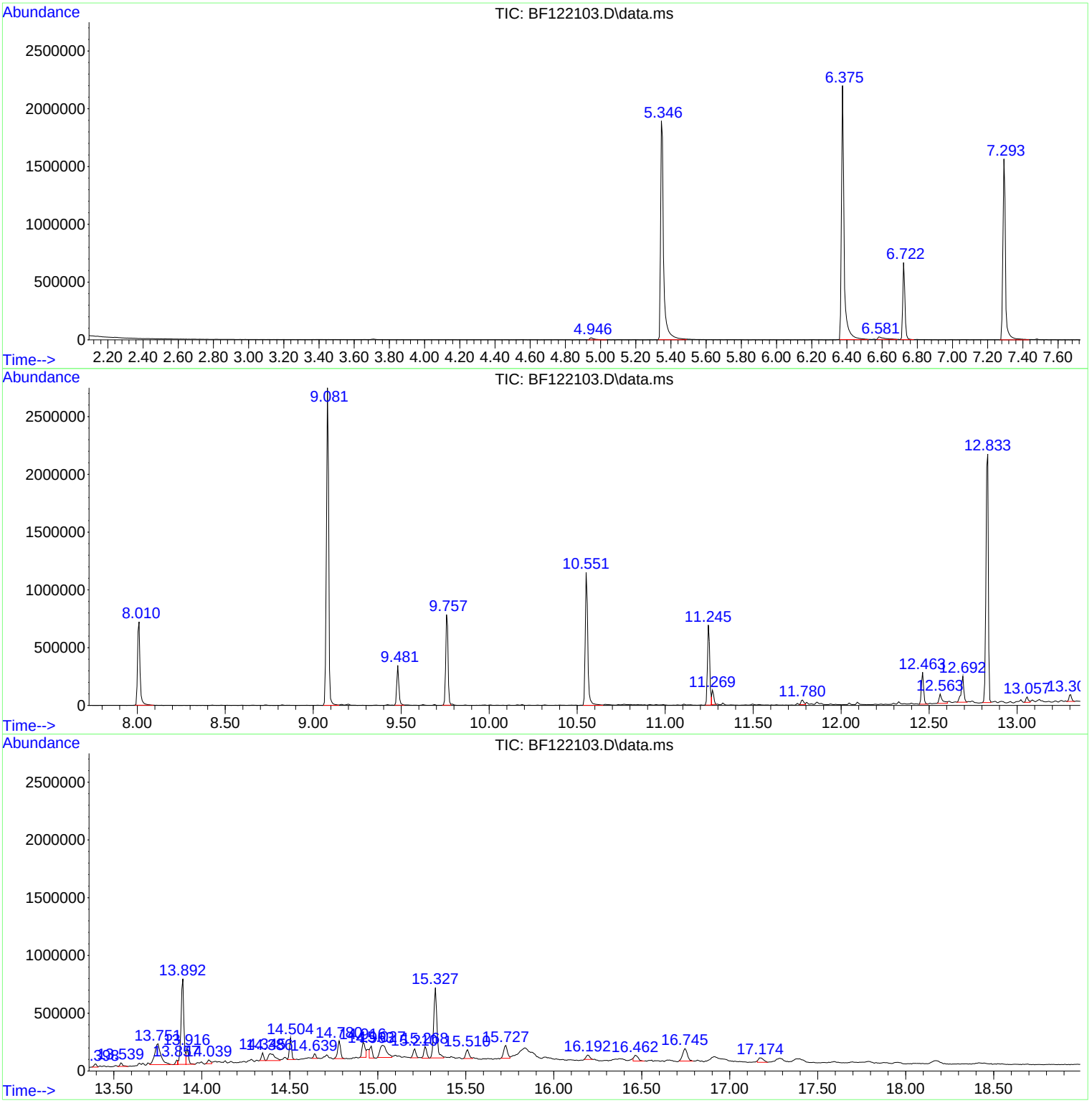
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

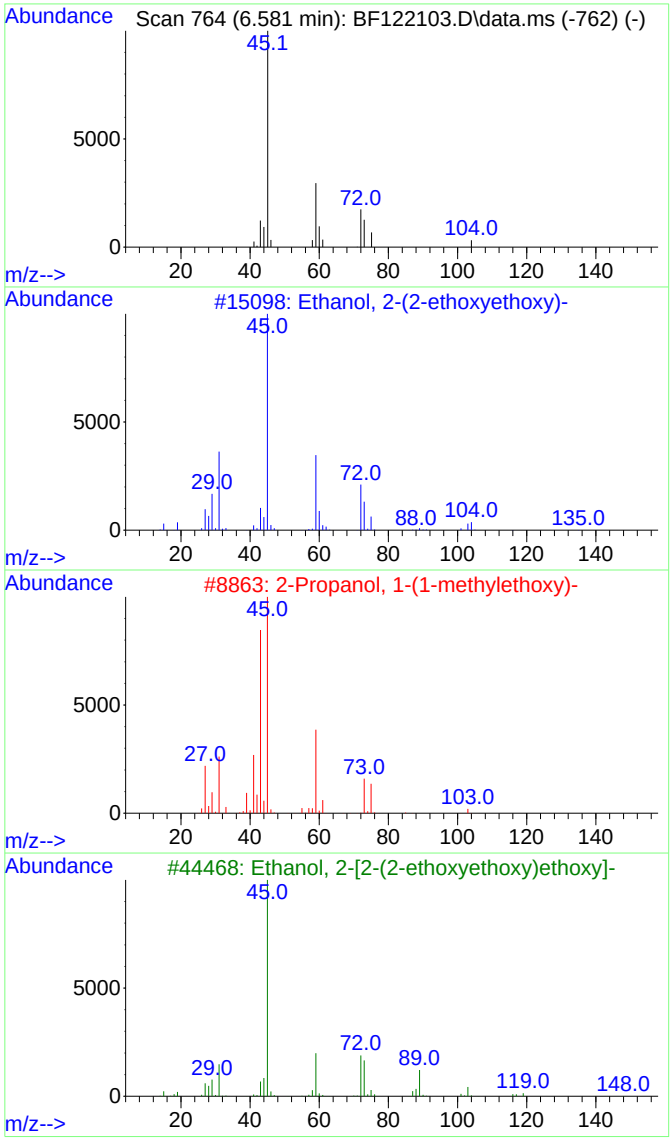
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

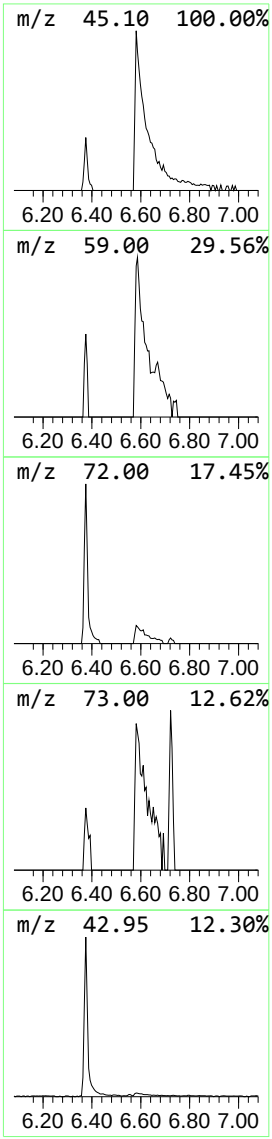
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	2.24 ng	63722	1,4-Dichlorobenzene-d4	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
4	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	38
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

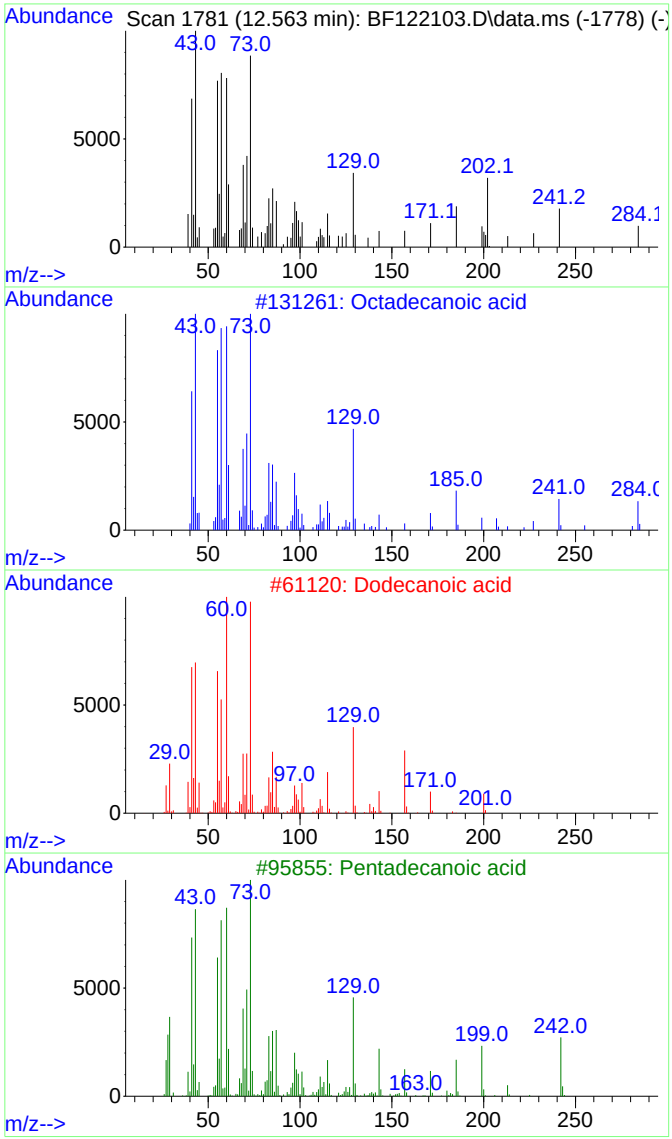
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

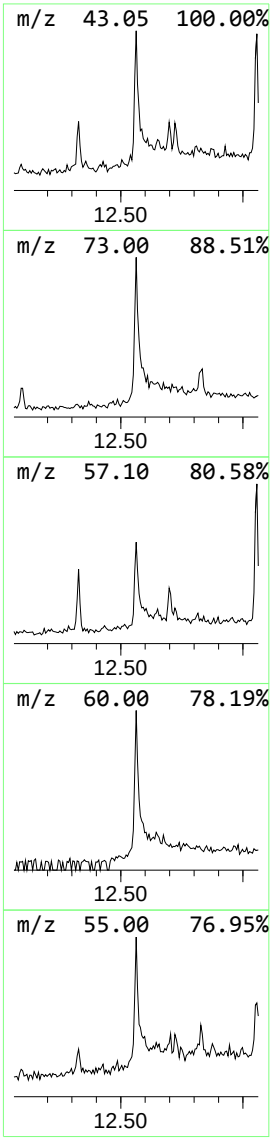
****

Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	3.27 ng	103640	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Dodecanoic acid	200	C12H24O2	000143-07-7	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

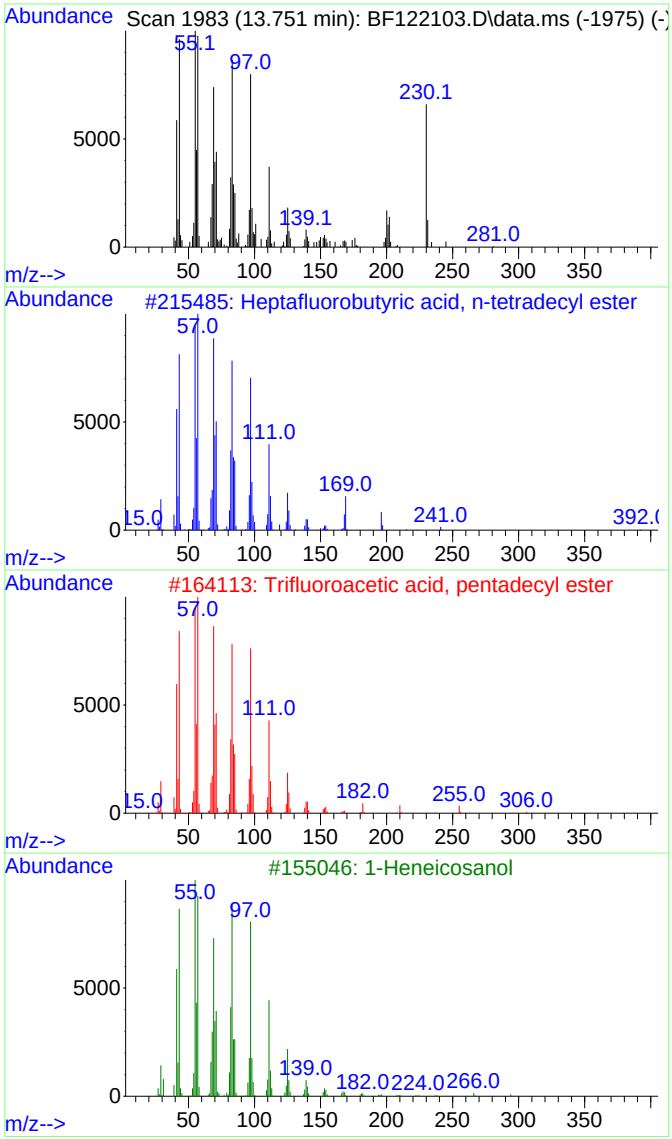
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

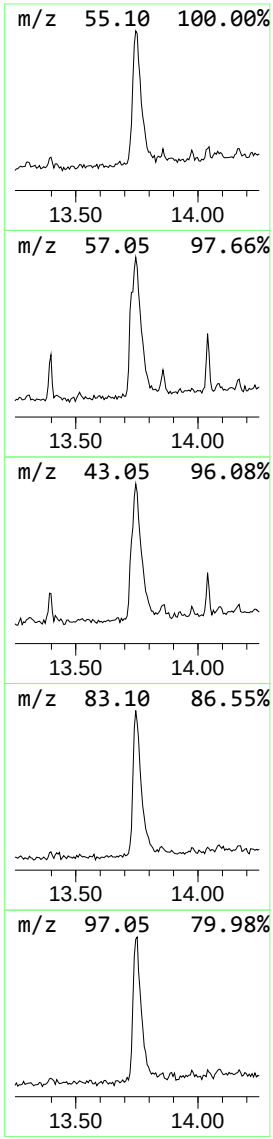
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptafluorobutyric acid, n-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	10.45 ng	438996	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

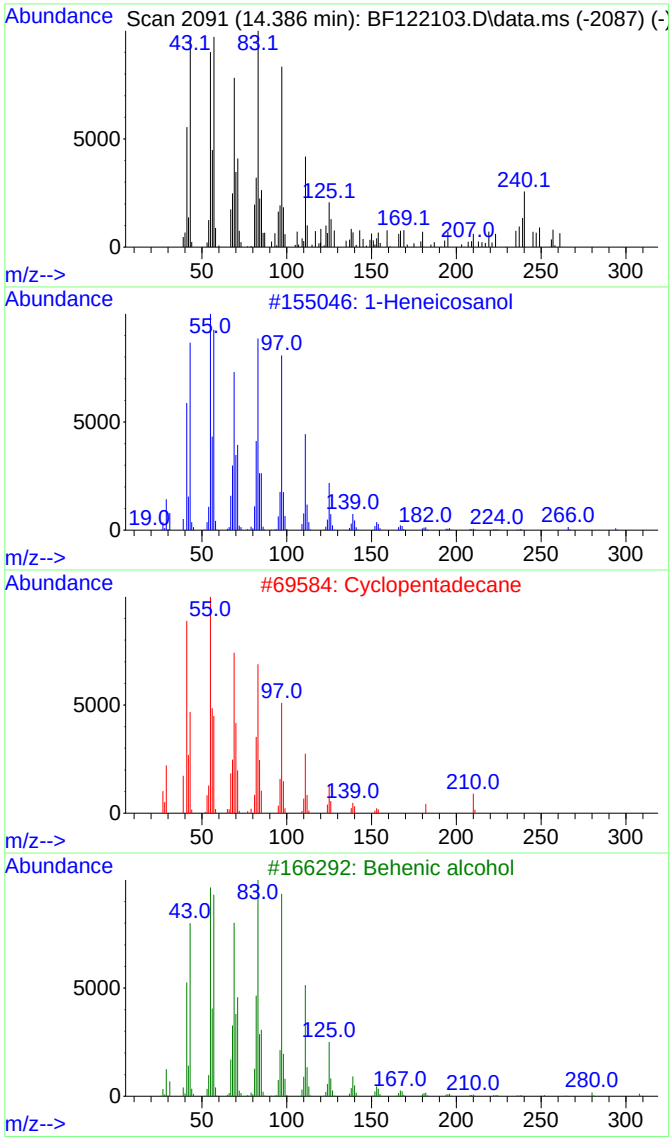
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

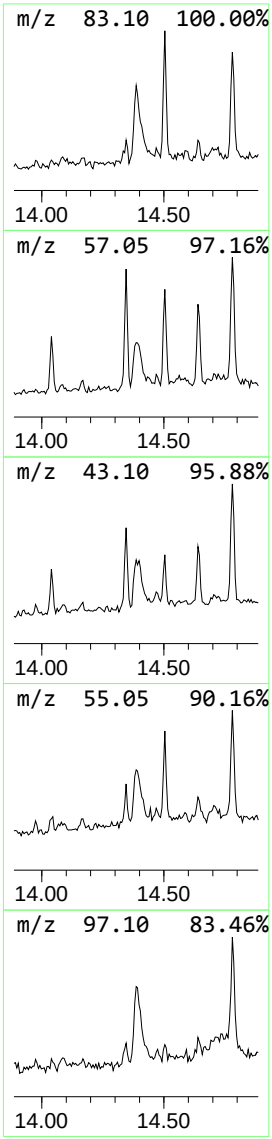
****

Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.386	3.78 ng	158698	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	17-Pentatriacontene	491	C35H70	006971-40-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

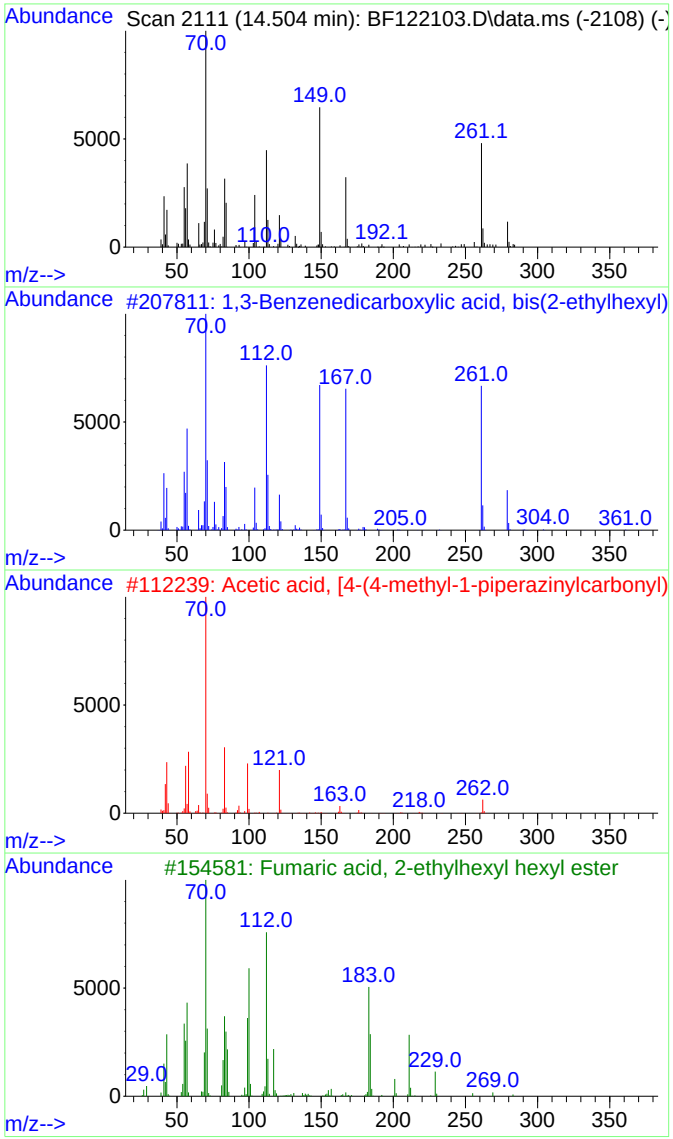
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

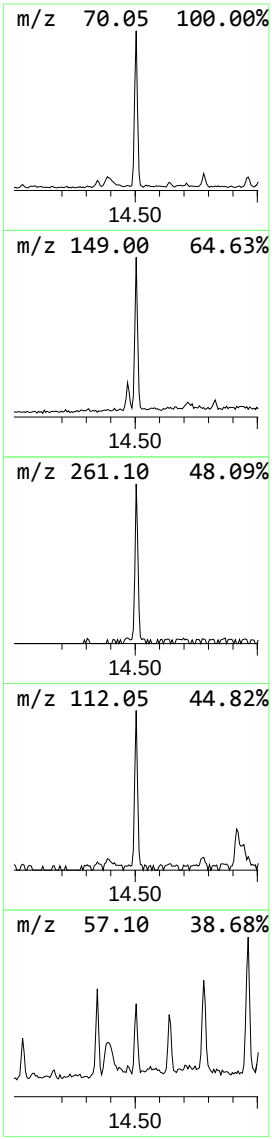
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	3.72 ng	156187	Chrysene-d12	13.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2	Acetic acid, [4-(4-methyl-1-pipe...	262	C14H18N2O3	346699-90-9	22
3	Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	22
4	Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	14
5	Diisooctyl phthalate	390	C24H38O4	000131-20-4	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

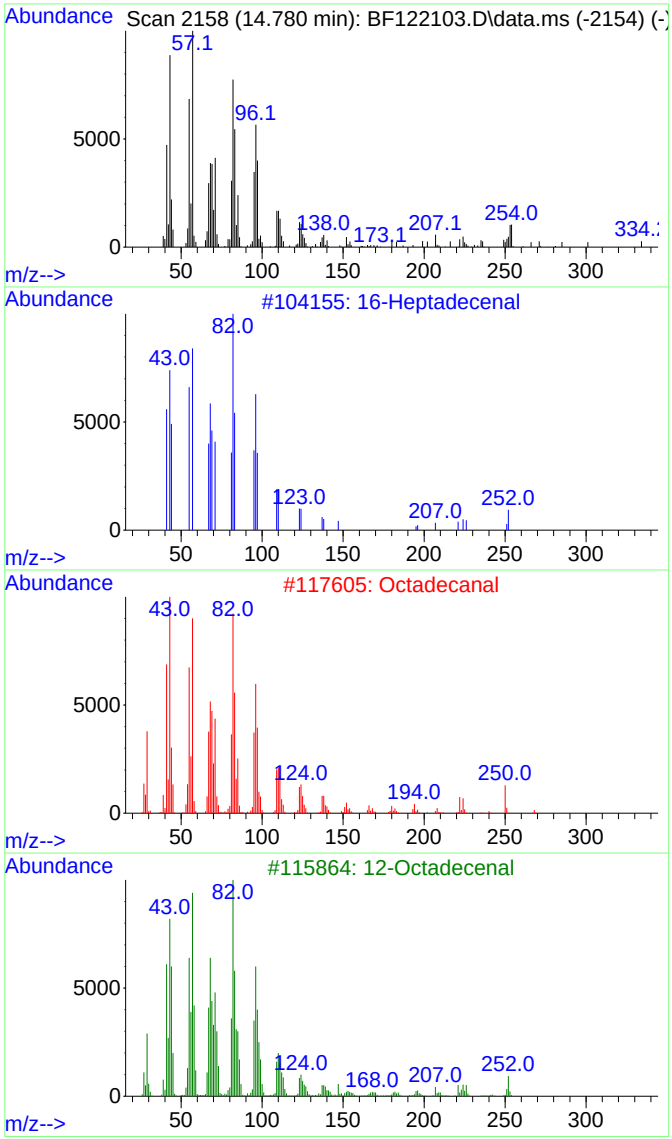
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

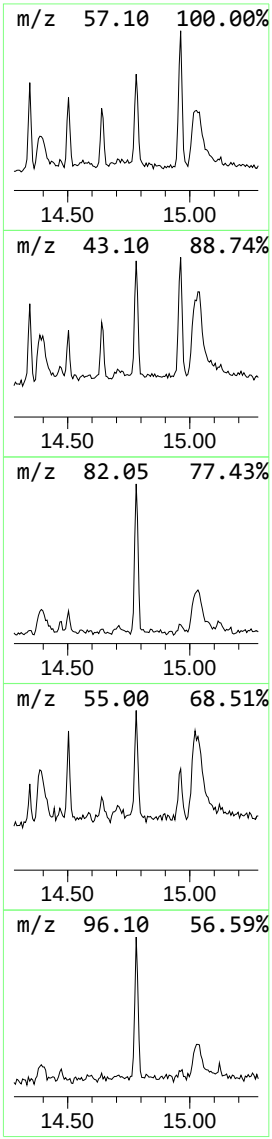
****

Peak Number 6 16-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	4.53 ng	170236	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1000144-57-9	93
2	Octadecanal	268	C18H36O	000638-66-4	91
3	12-Octadecenal	266	C18H34O	056554-91-7	90
4	13-Octadecenal	266	C18H34O	056554-90-6	90
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

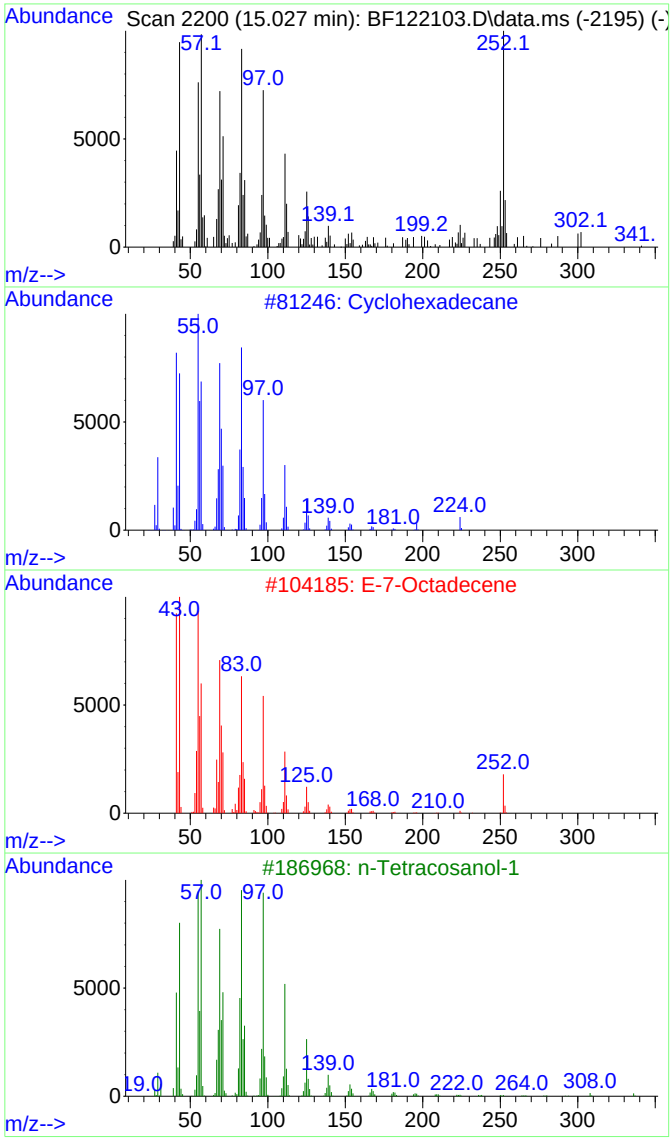
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

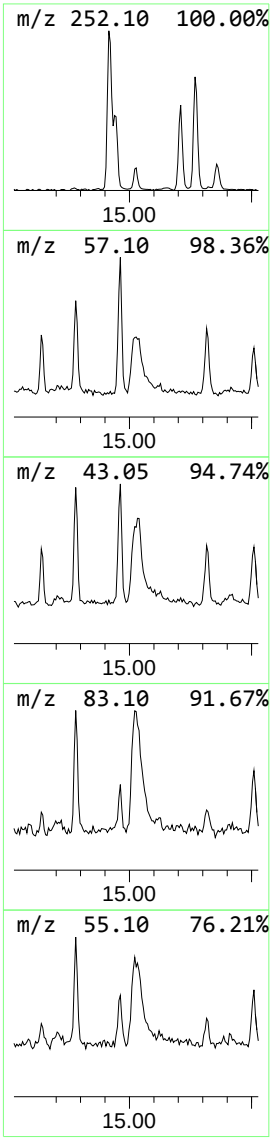
****

Peak Number 7 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	7.39 ng	277880	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	91
2	E-7-Octadecene	252	C18H36	1000130-92-0	89
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
4	1-Heptacosanol	396	C27H56O	002004-39-9	70
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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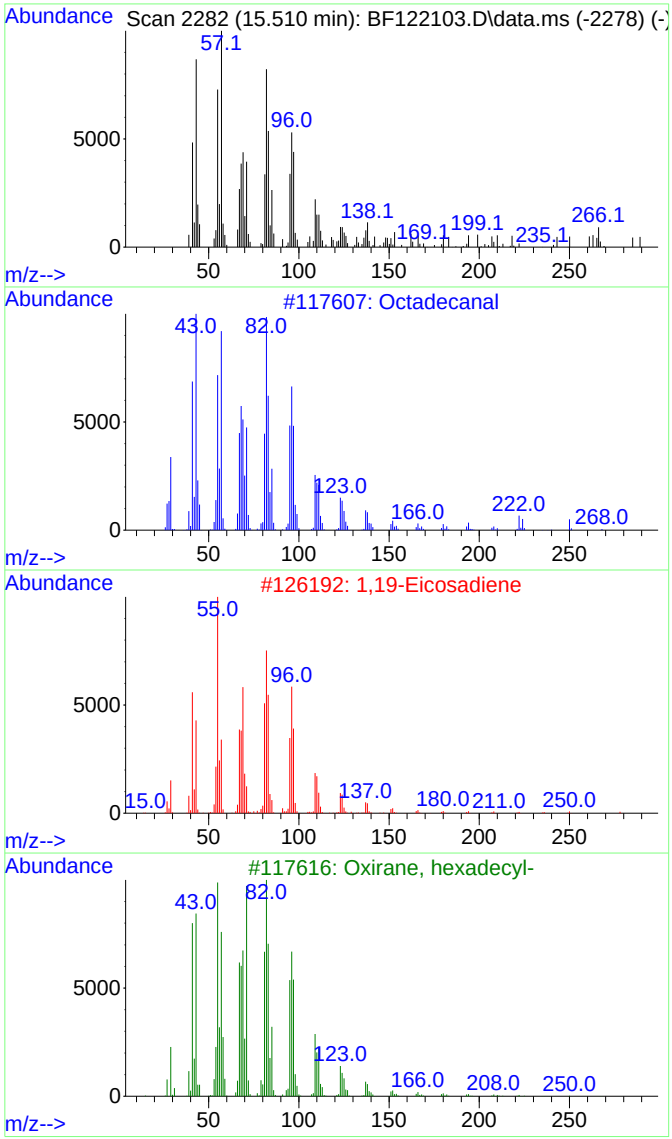
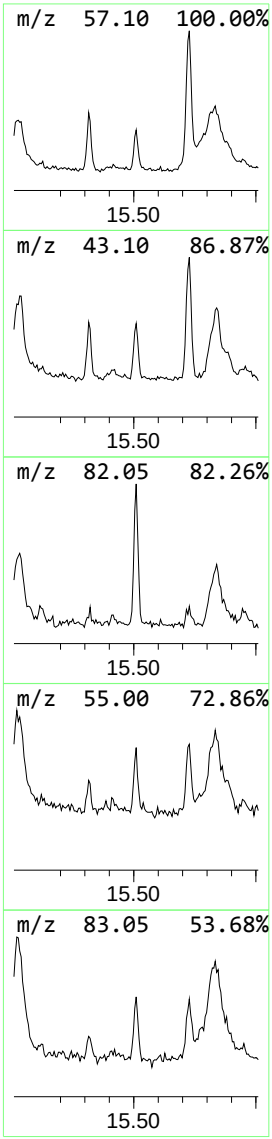
Peak Number 9 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.510	2.61 ng	98020	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	87
2	1,19-Eicosadiene	278	C20H38	014811-95-1	81
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
4	17-Octadecenal	266	C18H34O	056554-86-0	80
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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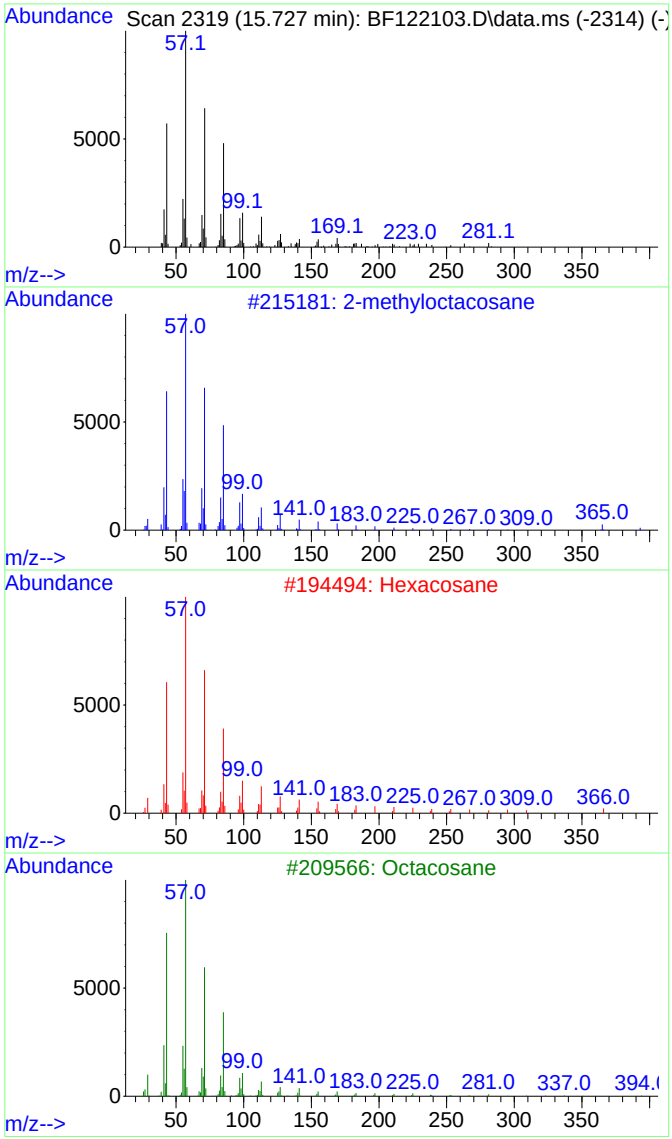
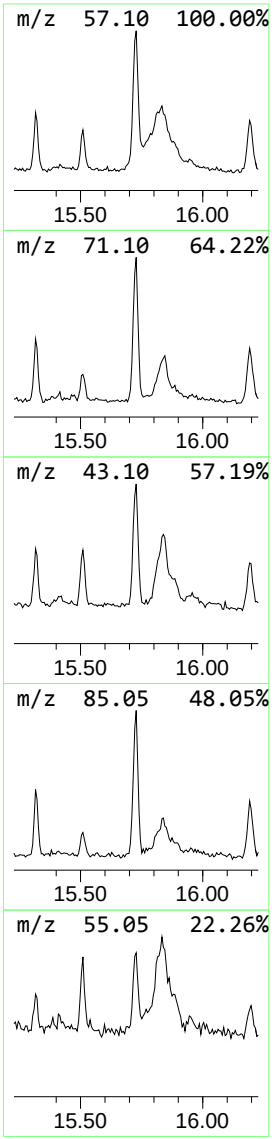
Peak Number 10 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.727	4.43 ng	166758	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

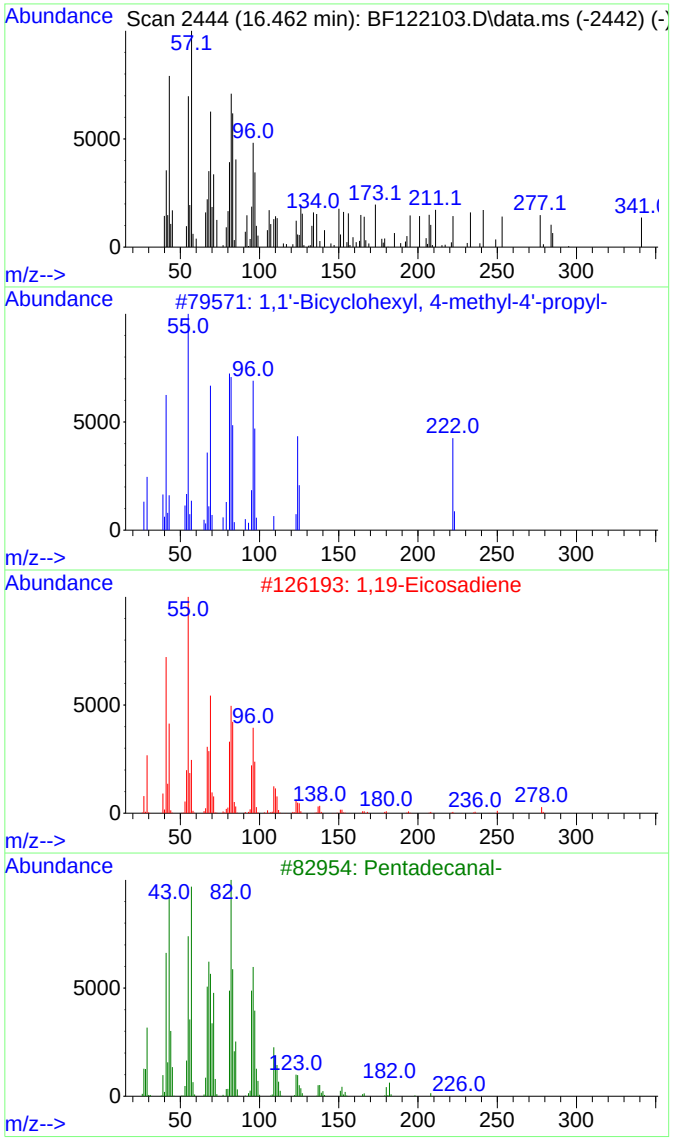
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

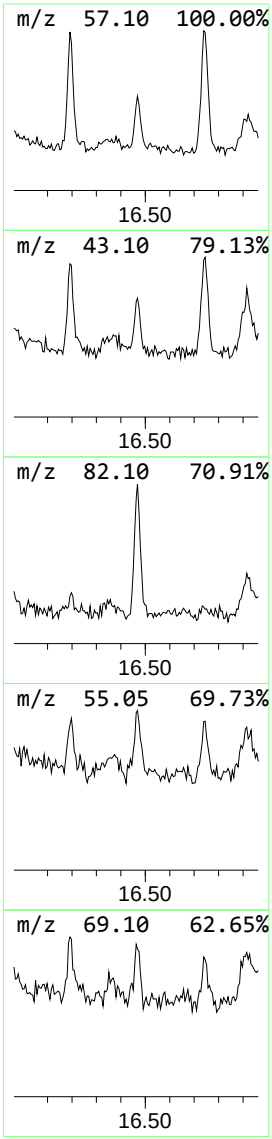
****

Peak Number 11 unknown16.46 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	2.07 ng	77975	Perylene-d12	15.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl, 4-methyl-4'-p...	222	C16H30	092343-70-9	18
2	1,19-Eicosadiene	278	C20H38	014811-95-1	15
3	Pentadecanal-	226	C15H30O	002765-11-9	14
4	Tetradecanal	212	C14H28O	000124-25-4	14
5	2-methylbutyric Acid, 2,2,2-trif...	184	C7H11F3O2	1000376-60-6	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102320\
Data File : BF122103.D
Acq On : 23 Oct 2020 17:19
Operator : JU/CG
Sample : L4436-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 35B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
Ethanol, 2-(2-e...	6.581	2.2	ng	63722	1	6.722	568793	20.0
Octadecanoic acid	12.563	3.3	ng	103640	4	11.245	633005	20.0
Heptafluorobuty...	13.751	10.4	ng	438996	5	13.892	840058	20.0
1-Heneicosanol	14.386	3.8	ng	158698	5	13.892	840058	20.0
1,3-Benzenedica...	14.504	3.7	ng	156187	5	13.892	840058	20.0
16-Heptadecenal	14.780	4.5	ng	170236	6	15.327	752367	20.0
Cyclohexadecane	15.027	7.4	ng	277880	6	15.327	752367	20.0
Octadecanal	15.510	2.6	ng	98020	6	15.327	752367	20.0
2-methyloctacosane	15.727	4.4	ng	166758	6	15.327	752367	20.0
unknown16.46	16.462	2.1	ng	77975	6	15.327	752367	20.0