LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

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: BF122193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	550	553	586	rBV	1576517	2154117	93.86%	11.558%
2	6.369	725	728	755	rBV	1860245	2295113	100.00%	12.314%
3	6.587	763	765	778	rBV2	25468	76773	3.35%	0.412%
4	6.710	783	786	798	rVB	617505	637262	27.77%	3.419%
5	7.281	880	883	902	rBV	1373629	1426562	62.16%	7.654%
6	7.992	1001	1004	1023	rVB	843805	843281	36.74%	4.525%
7	8.445	1078	1081	1102	rBV	35318	95515	4.16%	0.512%
8	9.069	1183	1187	1198	rBV	1753689	1801916	78.51%	9.668%
9	9.186	1203	1207	1213	rVB	51503	50089	2.18%	0.269%
10	9.469	1252	1255	1269	rVB	415817	380616	16.58%	2.042%
11	9.745	1298	1302	1314	rBV	1097253	991332	43.19%	5.319%
12	10.539	1433	1437	1452	rBV	1599658	1569764	68.40%	8.422%
13	11.233	1551	1555	1558	rBV	1099593	998797	43.52%	5.359%
14	11.257	1558	1559	1565	rVV	141754	131835	5.74%	0.707%
15	11.322	1568	1570	1575	rVB	20540	25430	1.11%	0.136%
16	11.763	1643	1645	1652	rVB3	84797	101516	4.42%	0.545%
17	11.857	1658	1661	1663	rBV	32037	30039	1.31%	0.161%
18	12.451	1759	1762	1768	rBV	281378	262681	11.45%	1.409%
19	12.680	1795	1801	1808	rVB	242854	264957	11.54%	1.422%
20	12.816	1820	1824	1827	rBV	1588449	1520468	66.25%	8.158%
21	12.904	1834	1839	1843	rVB4	16183	27642	1.20%	0.148%
22	13.016	1855	1858	1864	rVB2	34079	48547	2.12%	0.260%
23	13.121	1872	1876	1880	rBV3	21479	25772	1.12%	0.138%
24	13.657	1959	1967	1970	rBV3	23994	34075	1.48%	0.183%
25	13.710	1970	1976	1989	rBV3	250175	432398	18.84%	2.320%
26	13.880	2001	2005	2008	rBV2	804911	851749	37.11%	4.570%
27	13.910	2008	2010	2016	rVB	96680	108729	4.74%	0.583%
28	14.321	2076	2080	2083	rBV4	20449	26524	1.16%	0.142%
29	14.915	2177	2181	2184	rBV	84909	122304	5.33%	0.656%
30	14.939	2184	2185	2191	rVB	64683	62450	2.72%	0.335%
31	15.210	2227	2231	2235	rVB	37092	47896	2.09%	0.257%
32	15.268	2237	2241	2243	rVV	72159	82022	3.57%	0.440%
33	15.315	2246	2249	2261	rVB	452141	598684	26.09%	3.212%
34	15.692	2309	2313	2319	rVB	48659	69544	3.03%	0.373%
35	15.774	2323	2327	2333	rBV5	14743	33898	1.48%	0.182%
36	16.162	2388	2393	2397	rBV	45174	70776	3.08%	0.380%

LSC Area Percent Report

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Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

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	16.704	2479	2485	2489	rBV	35711	66266	2.89%	0.356%
38	16.756	2490	2494	2504	rVB3	39306	81853	3.57%	0.439%
39	17.186	2562	2567	2580	rVB	33473	90778	3.96%	0.487%
40	17.339	2589	2593	2602	rVB3	28151	57925	2.52%	0.311%
41	18.098	2718	2722	2735	rVB6	14987	39888	1.74%	0.214%

Sum of corrected areas: 18637783

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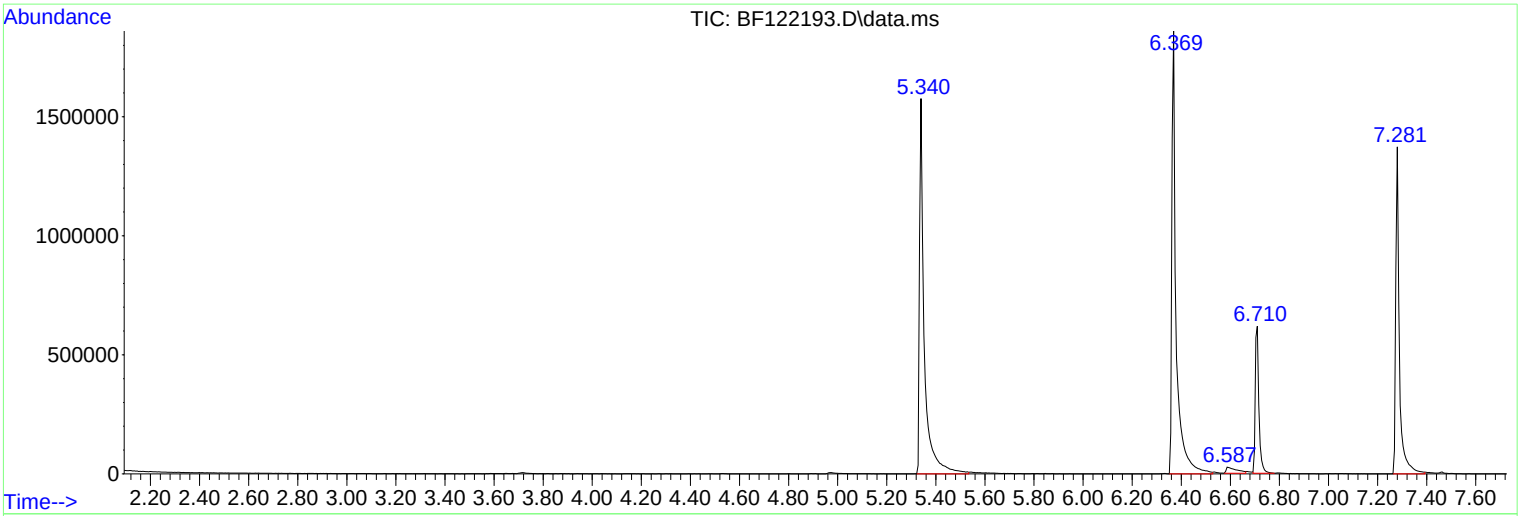
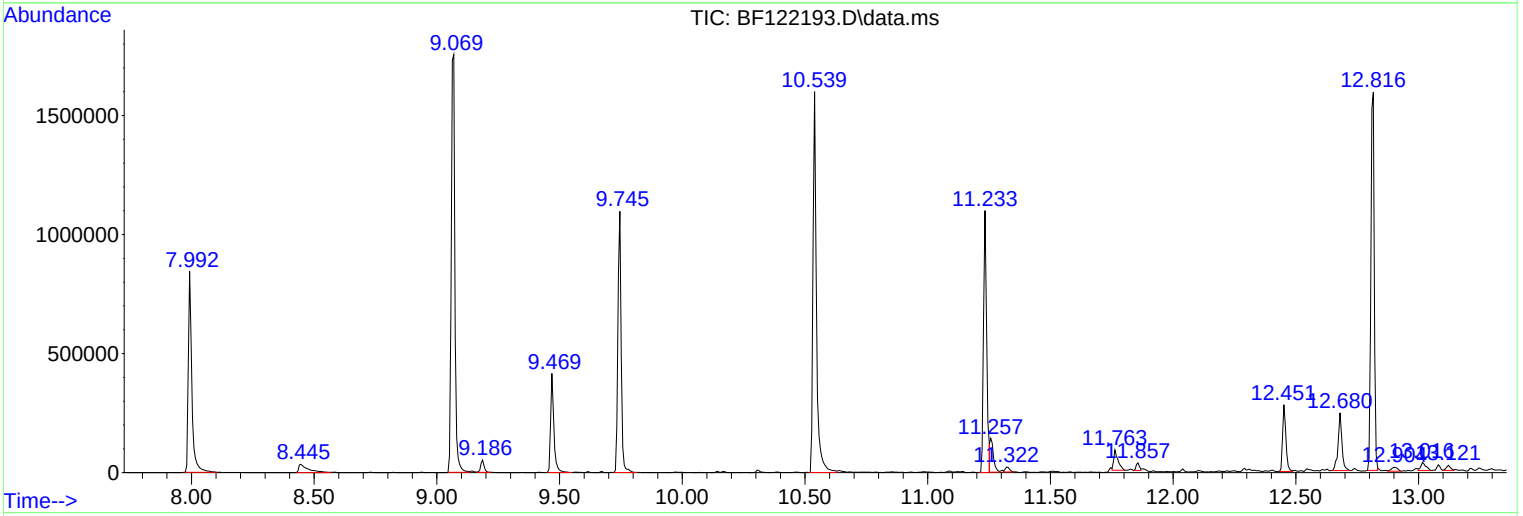
Misc :
ALS Vial : 16 Sample Multiplier: 1

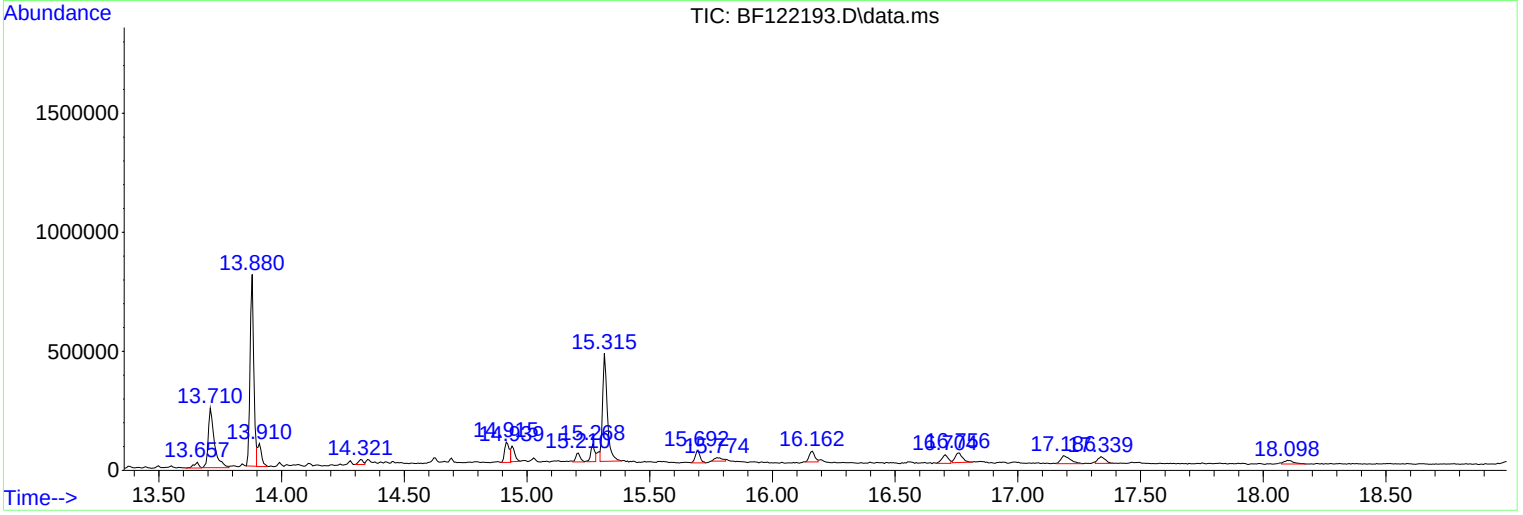
Instrument :
BNA_F
ClientSampleId :
2015

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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Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

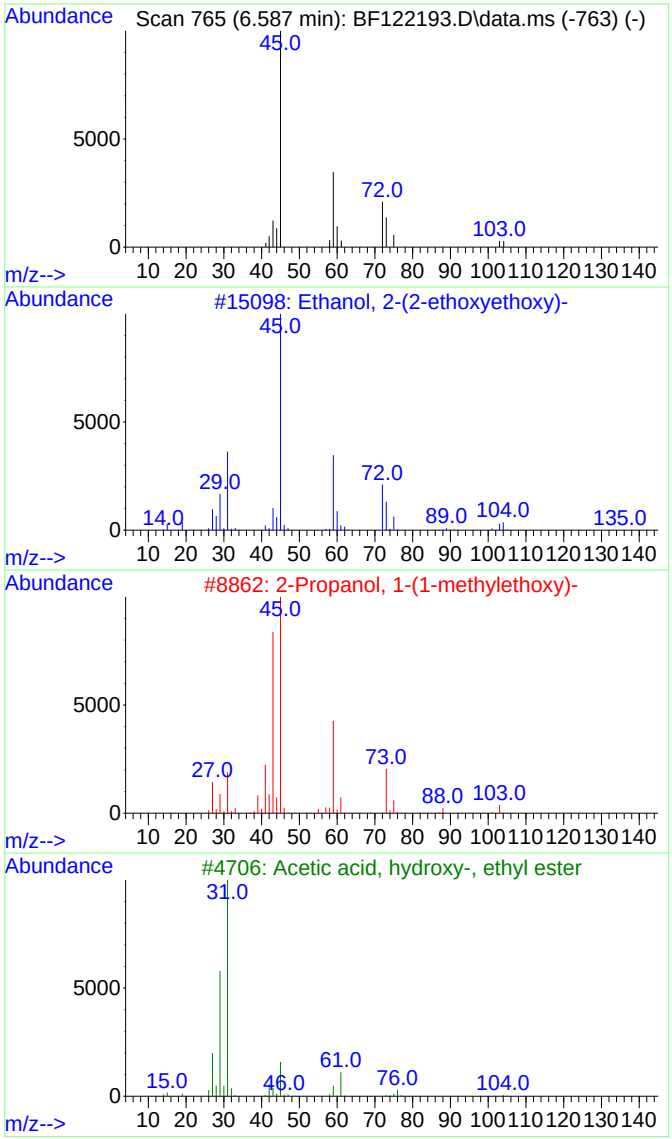
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

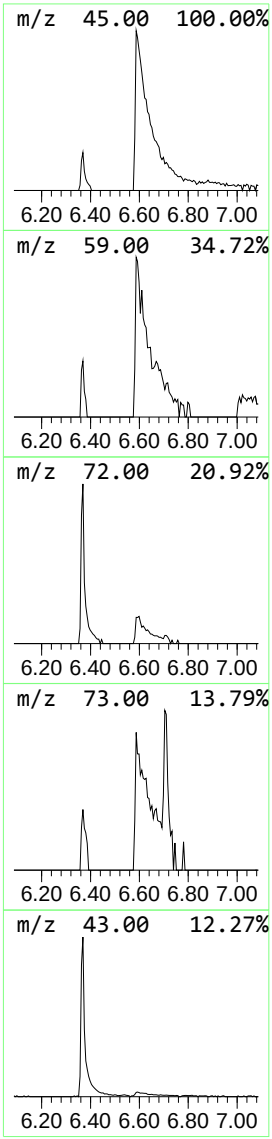
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.587	2.41 ng	76773	1,4-Dichlorobenzene-d4	6.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	9
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

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

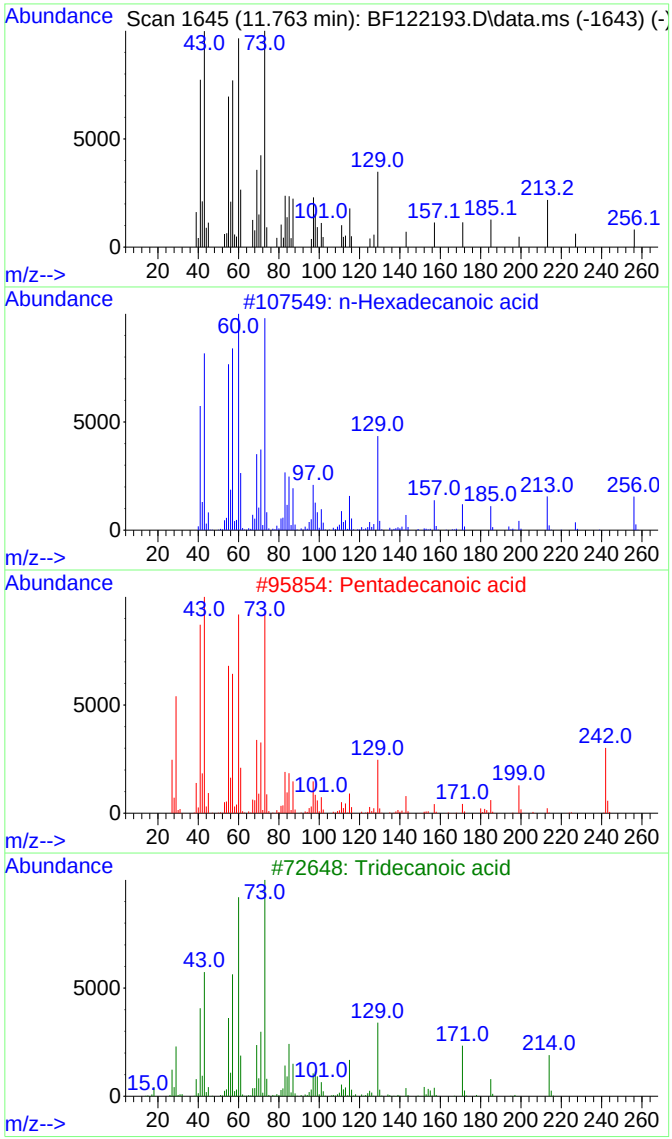
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

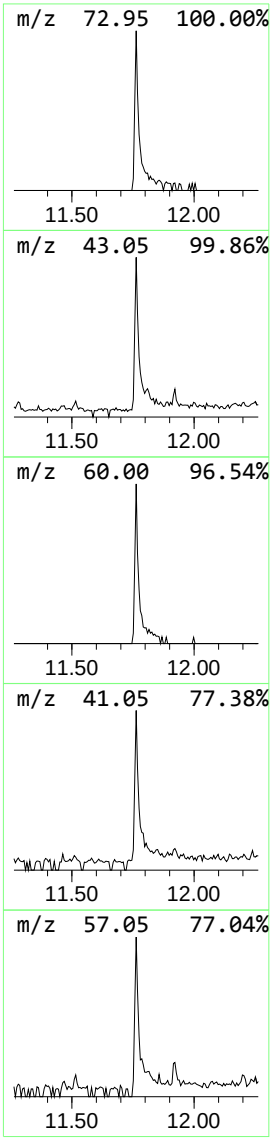
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	2.03 ng	101516	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

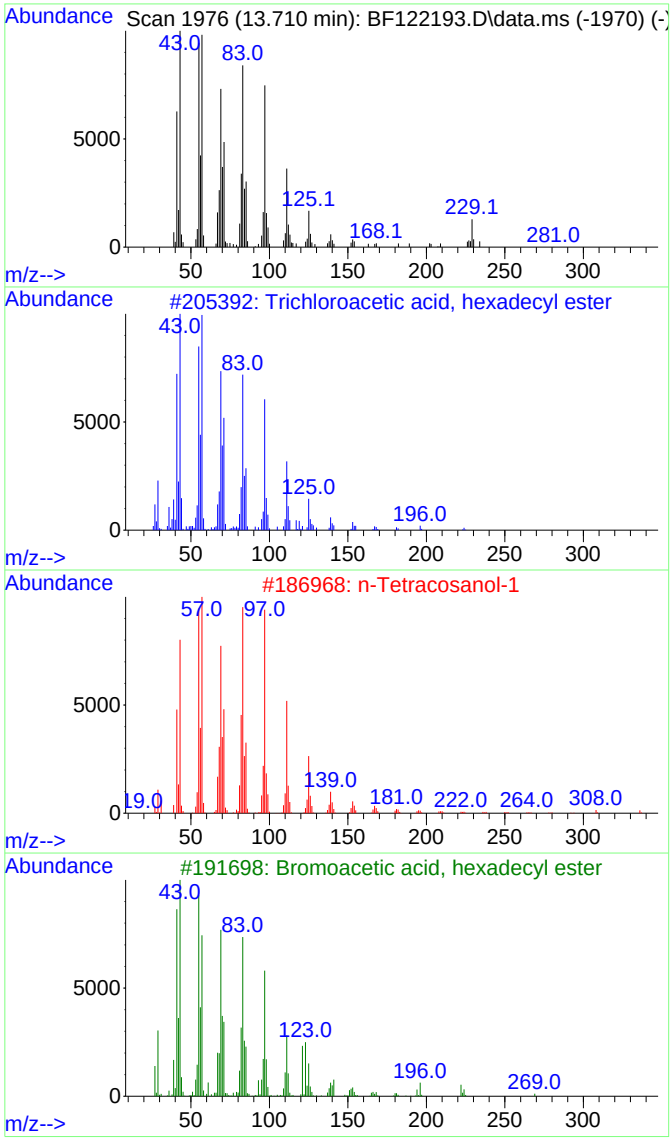
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

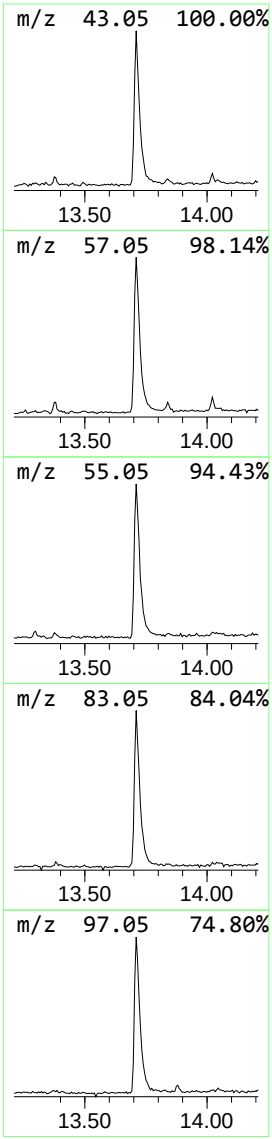
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	10.15 ng	432398	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

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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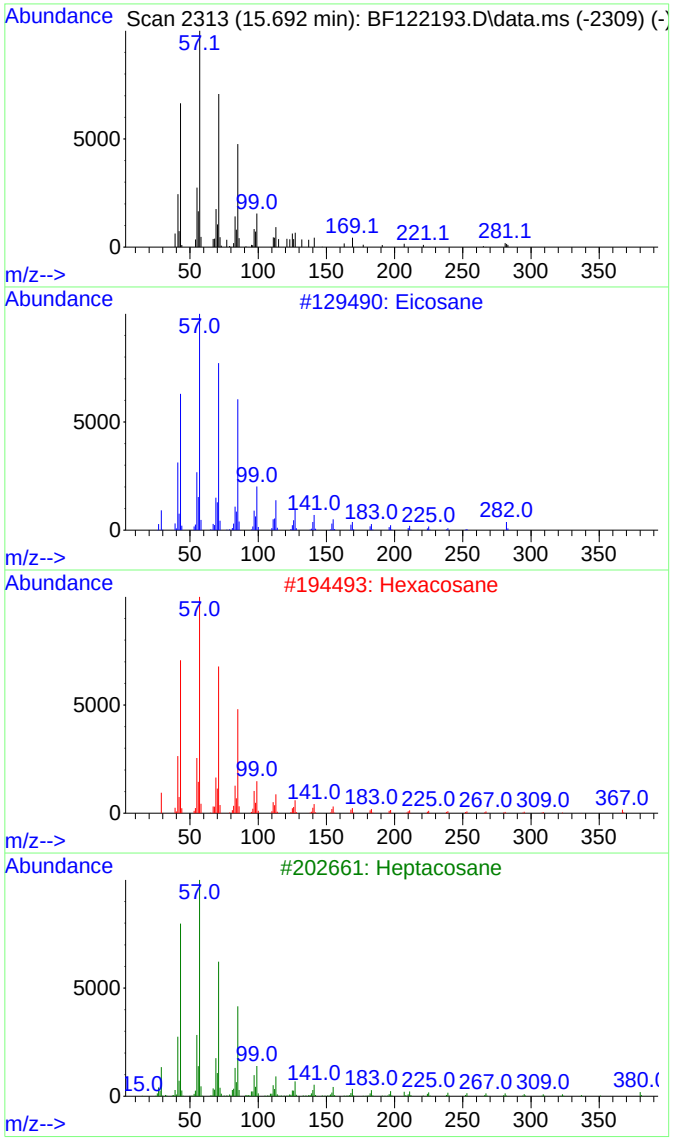
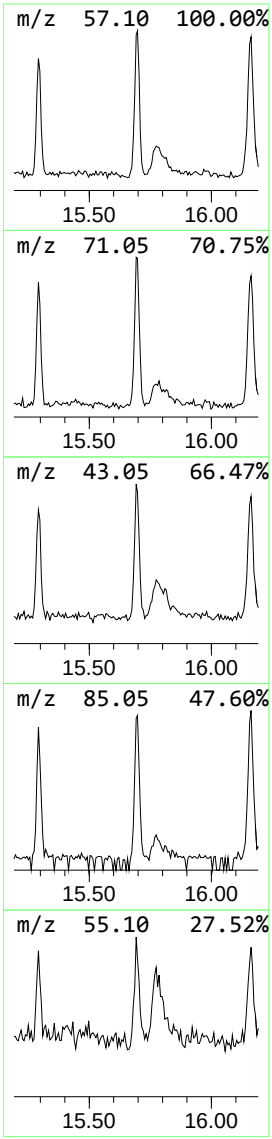
Peak Number 4 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.692	2.32 ng	69544	Perylene-d12	15.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2015

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

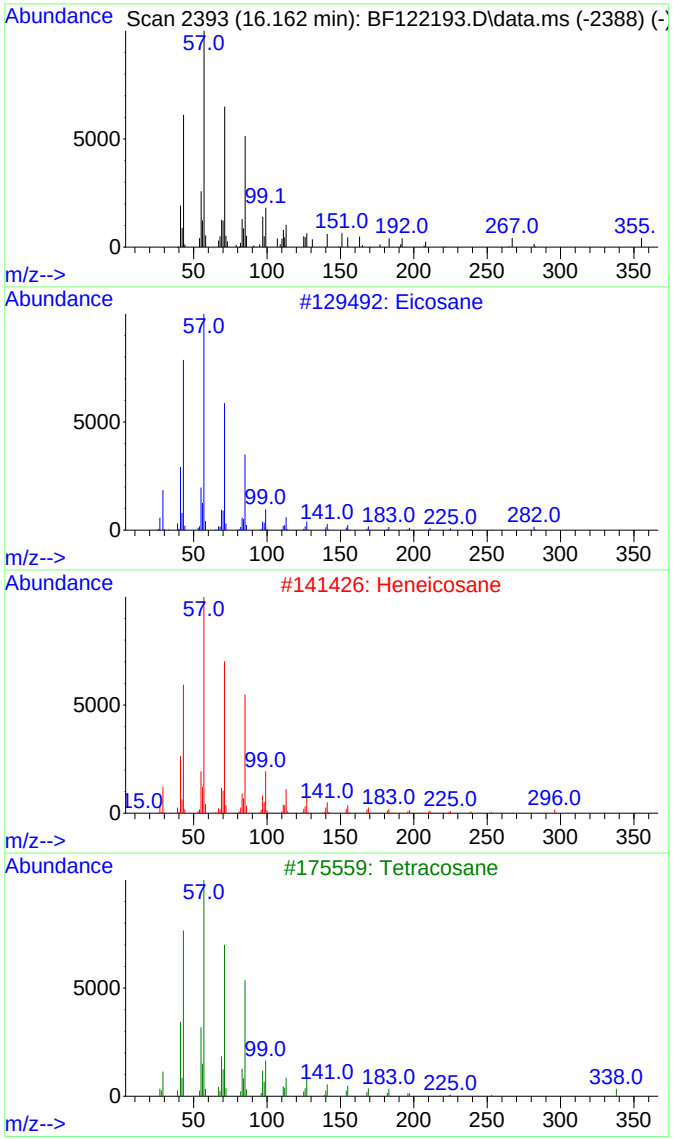
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

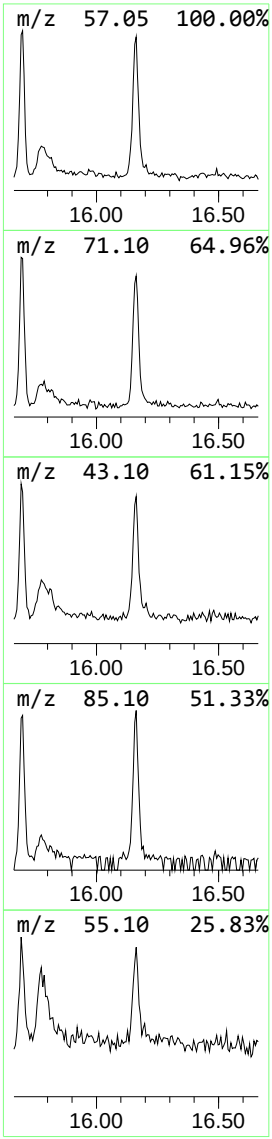
****

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.162	2.36 ng	70776	Perylene-d12	15.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heptadecane	240	C17H36	000629-78-7	83





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Acq On : 30 Oct 2020 21:51
Operator : JU/CG
Sample : L4541-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2015

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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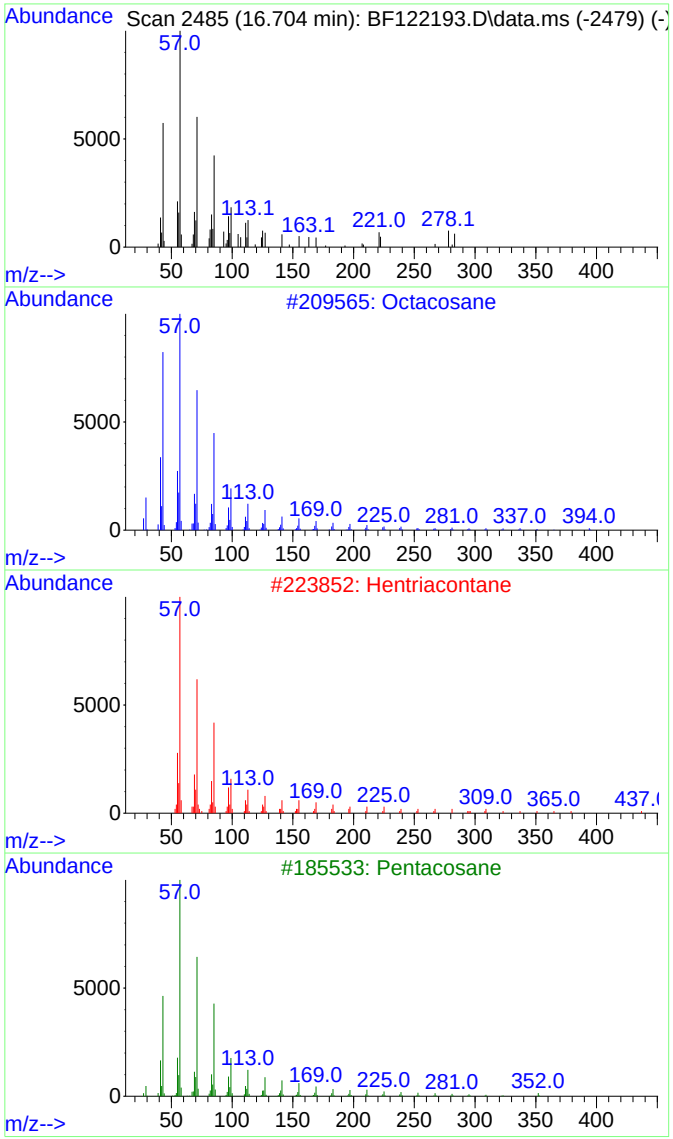
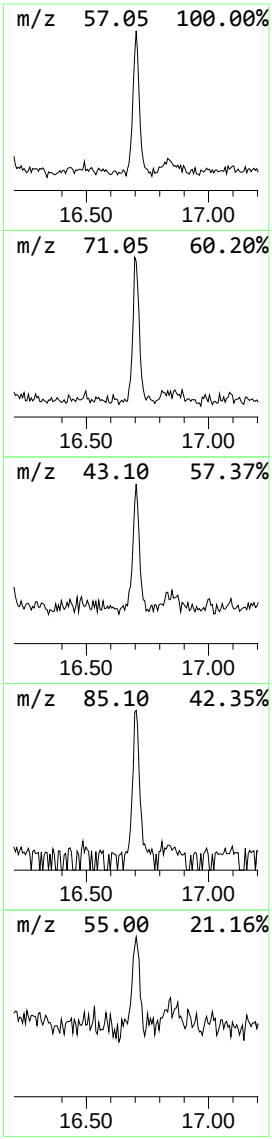
Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.703	2.21 ng	66266	Perylene-d12	15.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Tentatively Identified Compound (LSC) summary

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Data File : BF122193.D
Acq On : 30 Oct 2020 21:51
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Misc :
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Instrument : BNA_F
ClientSampleId : 2015

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...	6.587	2.4	ng	76773	1	6.710	637262	20.0
n-Hexadecanoic ...	11.763	2.0	ng	101516	4	11.233	998797	20.0
Trichloroacetic...	13.710	10.2	ng	432398	5	13.880	851749	20.0
Eicosane	15.692	2.3	ng	69544	6	15.315	598684	20.0
Heneicosane	16.162	2.4	ng	70776	6	15.315	598684	20.0
Octacosane	16.703	2.2	ng	66266	6	15.315	598684	20.0