LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

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-BF122921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	556	560	573	rBV	938332	830549	31.94%	5.334%
2	6.398	729	733	742	rBV	950084	872111	33.54%	5.601%
3	6.598	764	767	773	rBV2	26220	28243	1.09%	0.181%
4	6.763	792	795	799	rBV	575650	546534	21.02%	3.510%
5	7.334	886	892	895	rBV	1434204	1661099	63.88%	10.669%
6	7.957	993	998	1009	rBV	471627	485887	18.68%	3.121%
7	8.051	1009	1014	1017	rVB	796000	772387	29.70%	4.961%
8	9.133	1191	1198	1201	rBV	2363157	2600435	100.00%	16.702%
9	9.810	1307	1313	1316	rBV	834965	836276	32.16%	5.371%
10	10.598	1440	1447	1455	rBV	1088873	1028322	39.54%	6.605%
11	11.292	1561	1565	1569	rVV	875171	808327	31.08%	5.192%
12	11.363	1572	1577	1579	rVB3	28184	26408	1.02%	0.170%
13	11.692	1628	1633	1637	rVB	75252	72899	2.80%	0.468%
14	11.833	1653	1657	1670	rBV2	134468	167738	6.45%	1.077%
15	12.398	1744	1753	1756	rVB2	40032	50746	1.95%	0.326%
16	12.621	1788	1791	1800	rBV	47787	62068	2.39%	0.399%
17	12.786	1817	1819	1824	rVB	52527	39691	1.53%	0.255%
18	12.886	1831	1836	1839	rBV	2084716	1941456	74.66%	12.470%
19	13.121	1871	1876	1883	rBV	53285	52334	2.01%	0.336%
20	13.351	1909	1915	1922	rBV4	33816	46764	1.80%	0.300%
21	13.463	1932	1934	1937	rVB	63454	47082	1.81%	0.302%
22	13.792	1986	1990	2001	rBV	249163	359707	13.83%	2.310%
23	13.939	2010	2015	2018	rBV	726994	675560	25.98%	4.339%
24	14.110	2041	2044	2047	rBV	91614	79965	3.08%	0.514%
25	14.421	2093	2097	2099	rBV	88138	84122	3.23%	0.540%
26	14.574	2120	2123	2126	rBV	28568	27022	1.04%	0.174%
27	14.698	2141	2144	2146	rBV	45546	44944	1.73%	0.289%
28	14.721	2146	2148	2151	rVB	95213	81434	3.13%	0.523%
29	15.051	2199	2204	2208	rBV	89190	99492	3.83%	0.639%
30	15.380	2255	2260	2264	rBV	476855	579389	22.28%	3.721%
31	15.415	2264	2266	2275	rVB	85620	108944	4.19%	0.700%
32	15.839	2333	2338	2344	rBV	72930	109389	4.21%	0.703%
33	16.327	2415	2421	2428	rBV3	67265	120907	4.65%	0.777%
34	16.898	2511	2518	2526	rBV2	36851	74798	2.88%	0.480%
35	17.392	2597	2602	2611	rVB10	9744	28850	1.11%	0.185%
36	17.580	2626	2634	2641	rVB2	28199	68784	2.65%	0.442%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

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-BF122921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.380	2763	2770	2780	rVB5	17112	48870	1.88%	0.314%

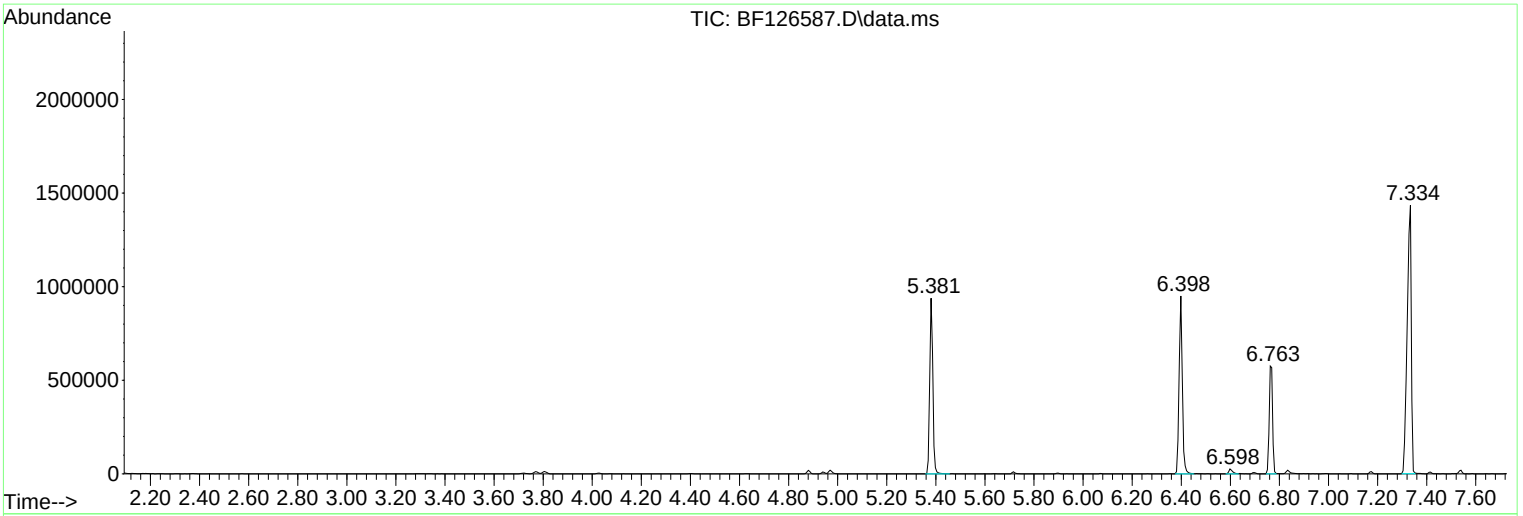
Sum of corrected areas: 15569533

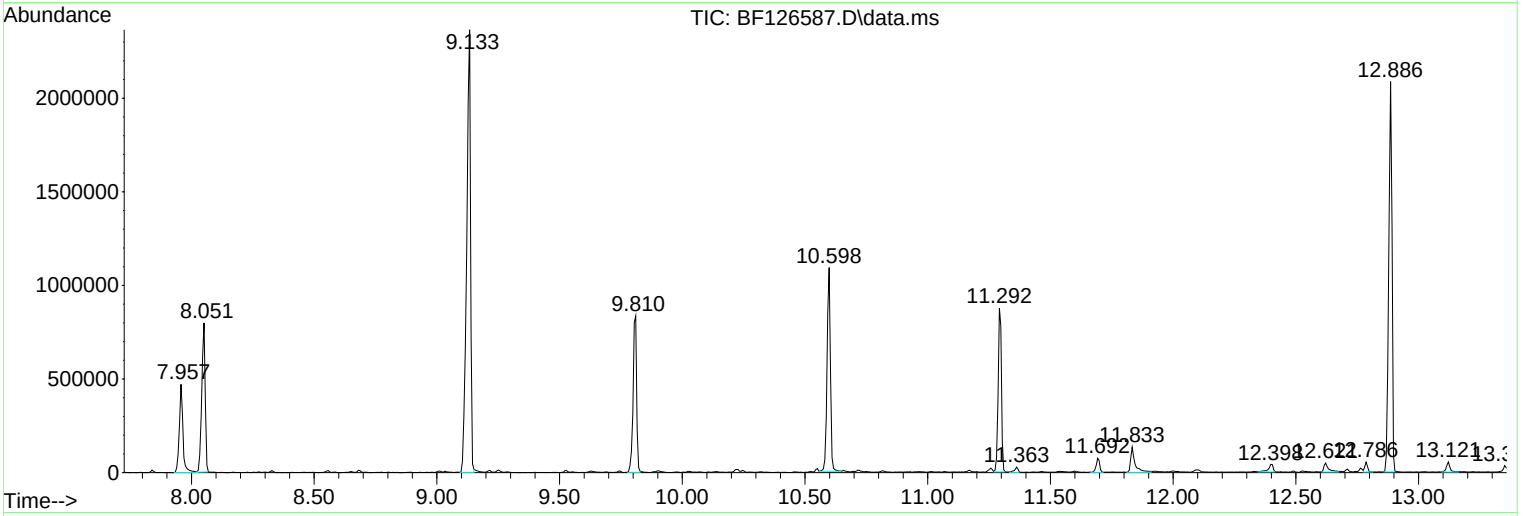
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

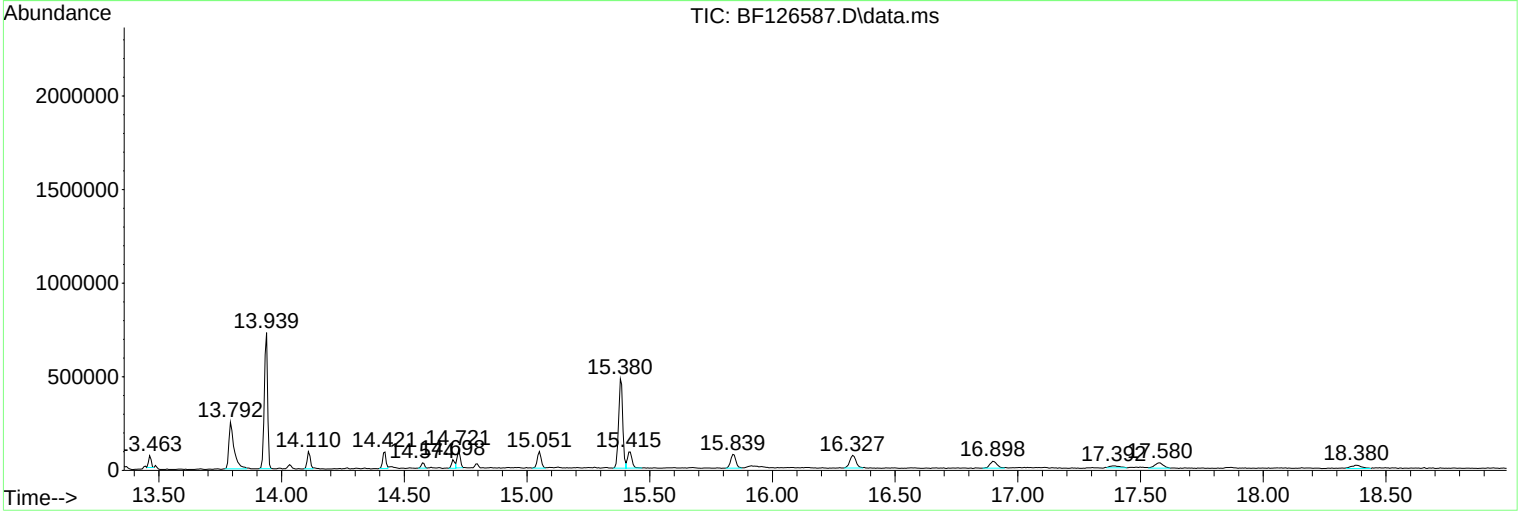
Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

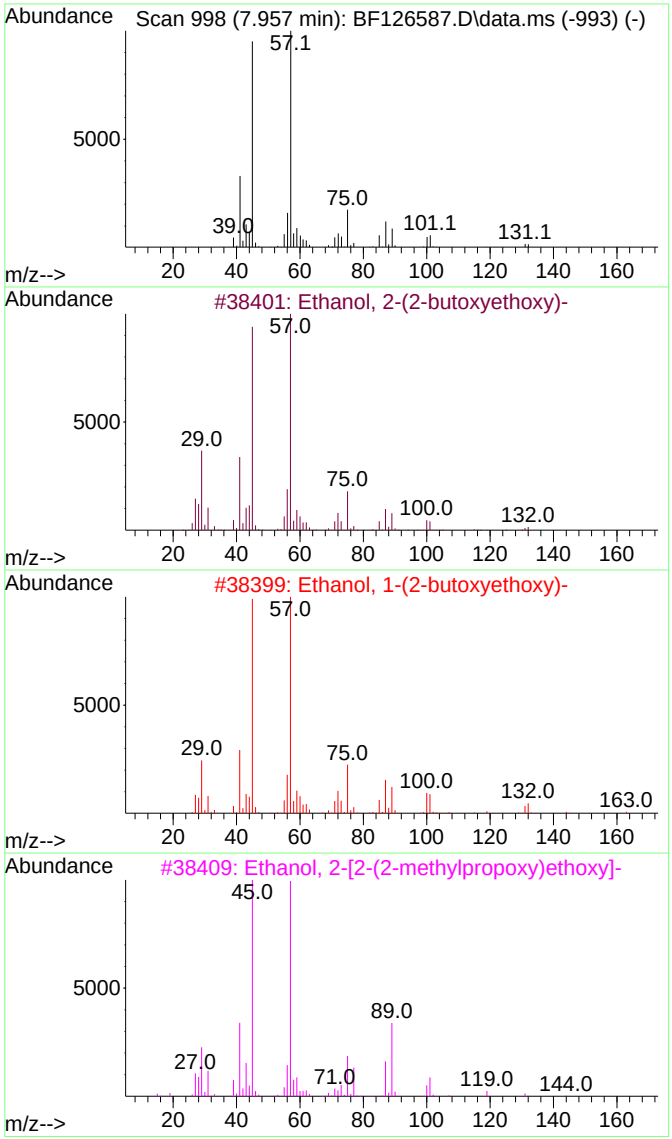
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

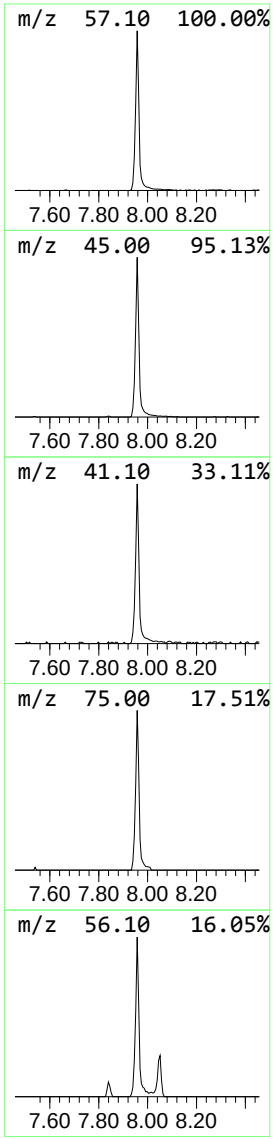
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	12.58 ng	485887	Naphthalene-d8	8.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butyl lactate	146	C7H14O3	000138-22-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

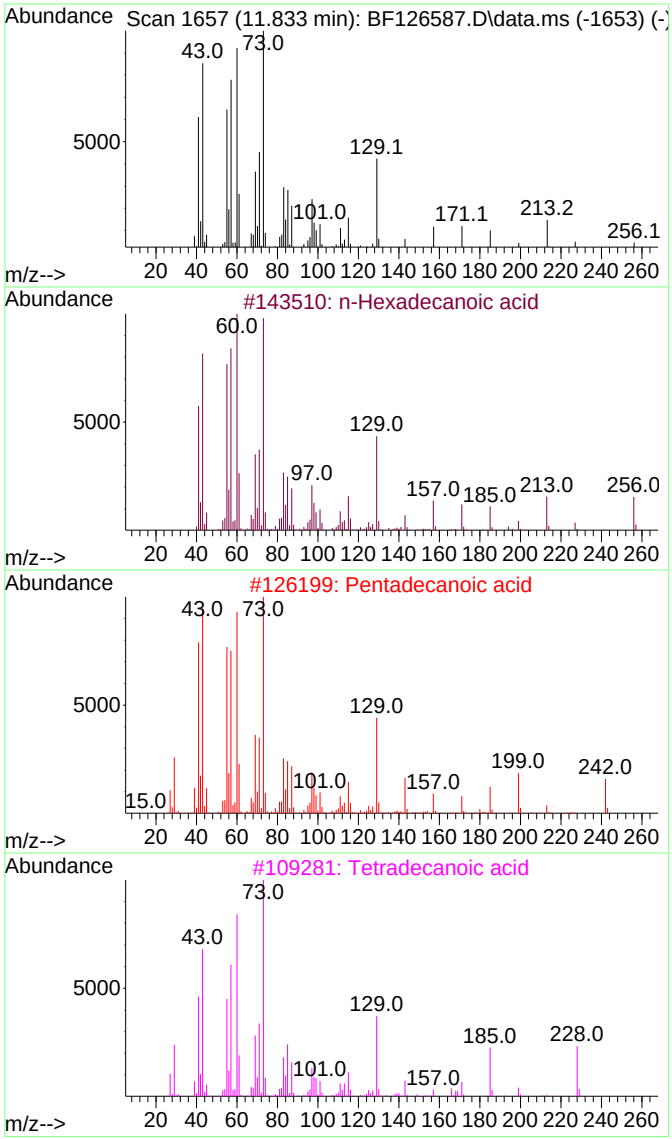
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

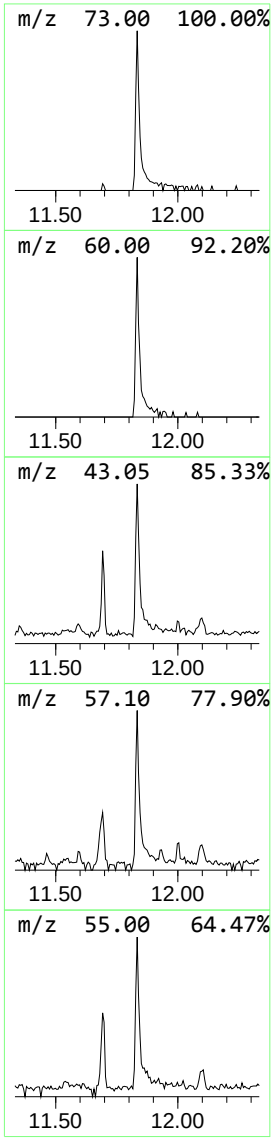
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	4.15 ng	167738	Phenanthrene-d10	11.292

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

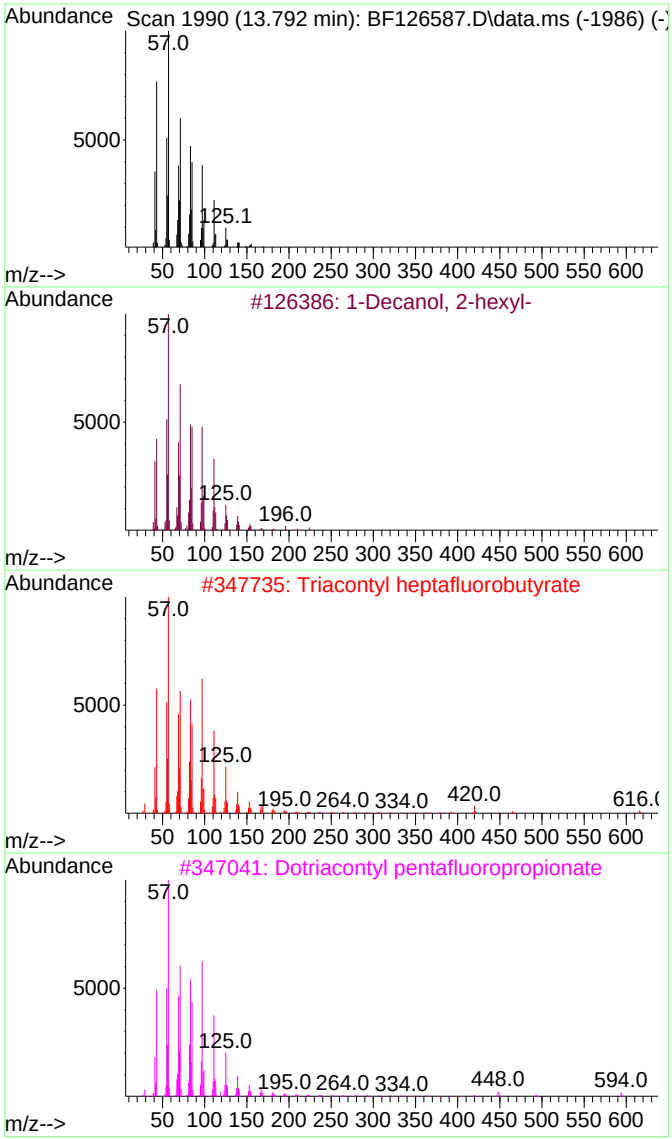
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

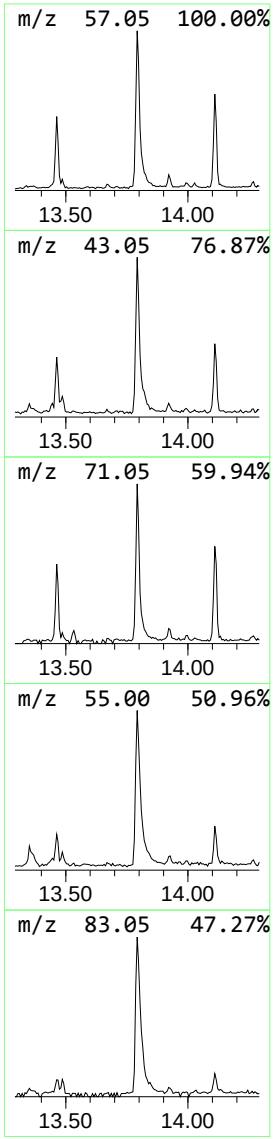
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Decanol, 2-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	10.65 ng	359707	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2	Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	90
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	90
4	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	90
5	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

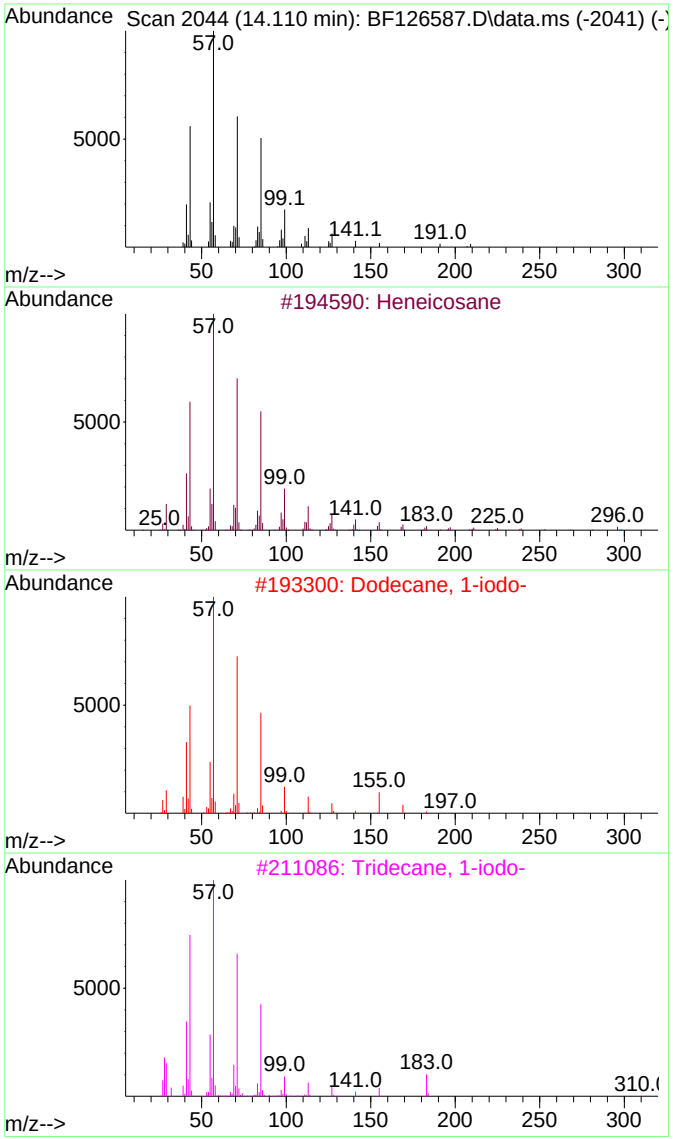
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

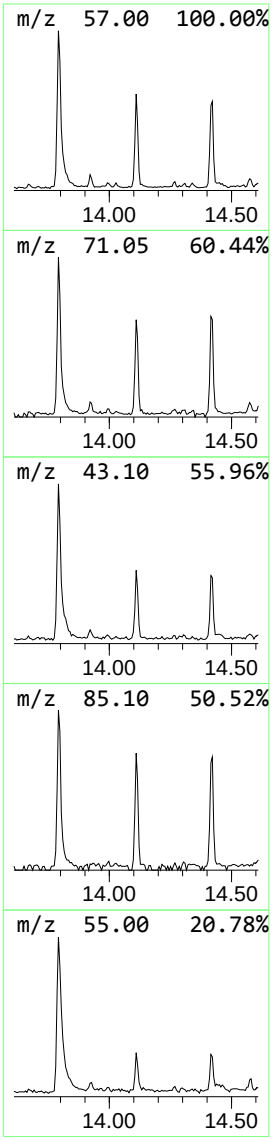
****

Peak Number 4 Dodecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.37 ng	79965	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Hexadecane	226	C16H34	000544-76-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

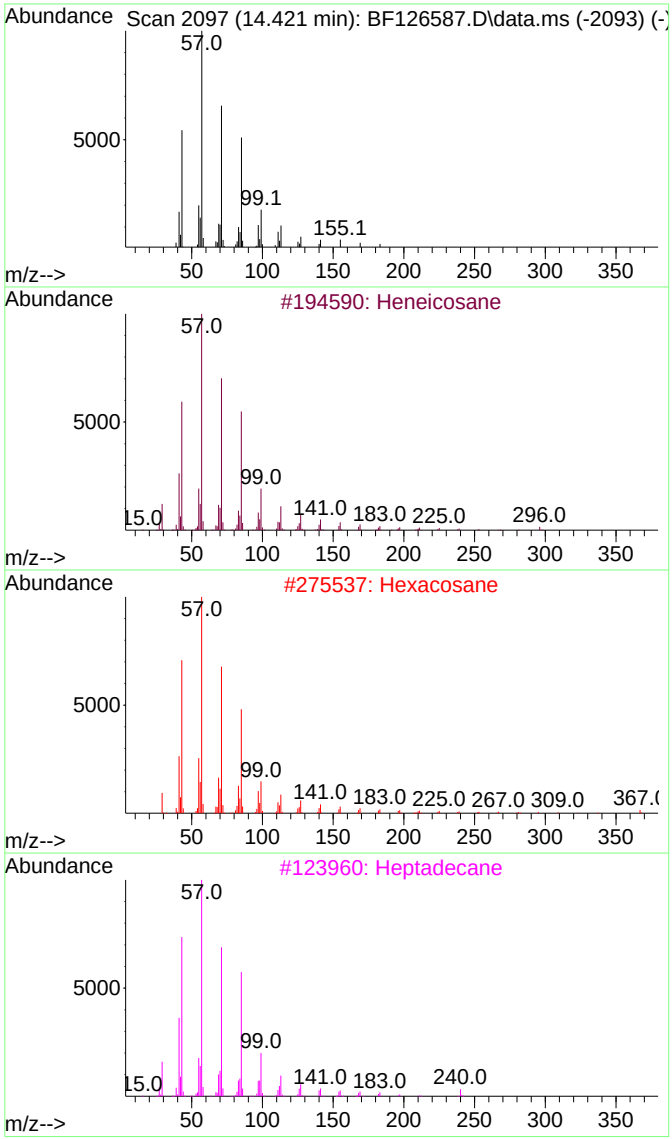
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

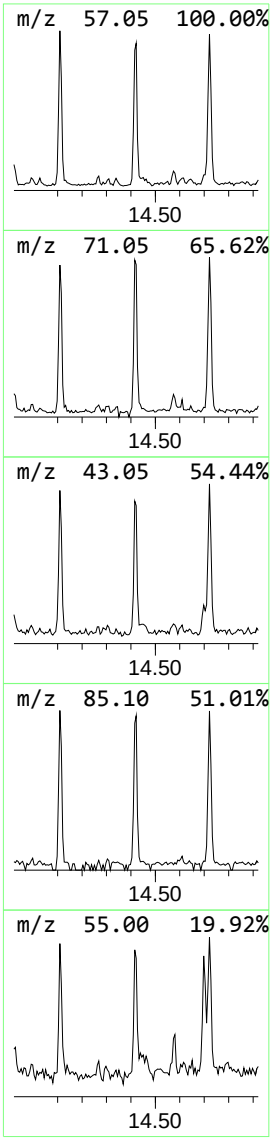
****

Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.421	2.49 ng	84122	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	2-Methyltetracosane	352	C25H52	001560-78-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

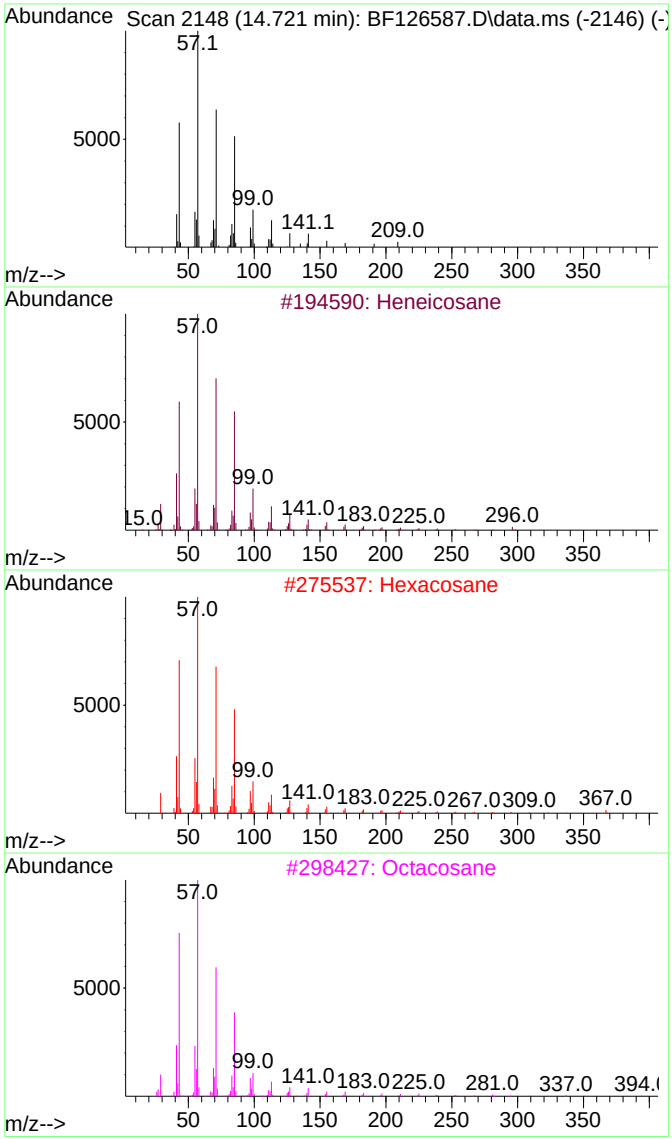
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

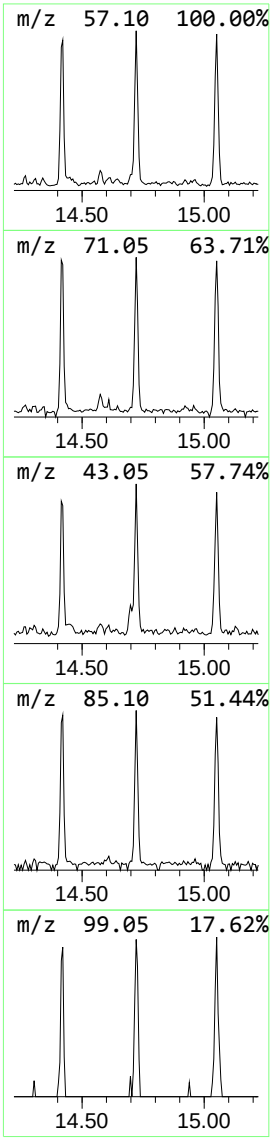
****

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.81 ng	81434	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Docosane	310	C22H46	000629-97-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

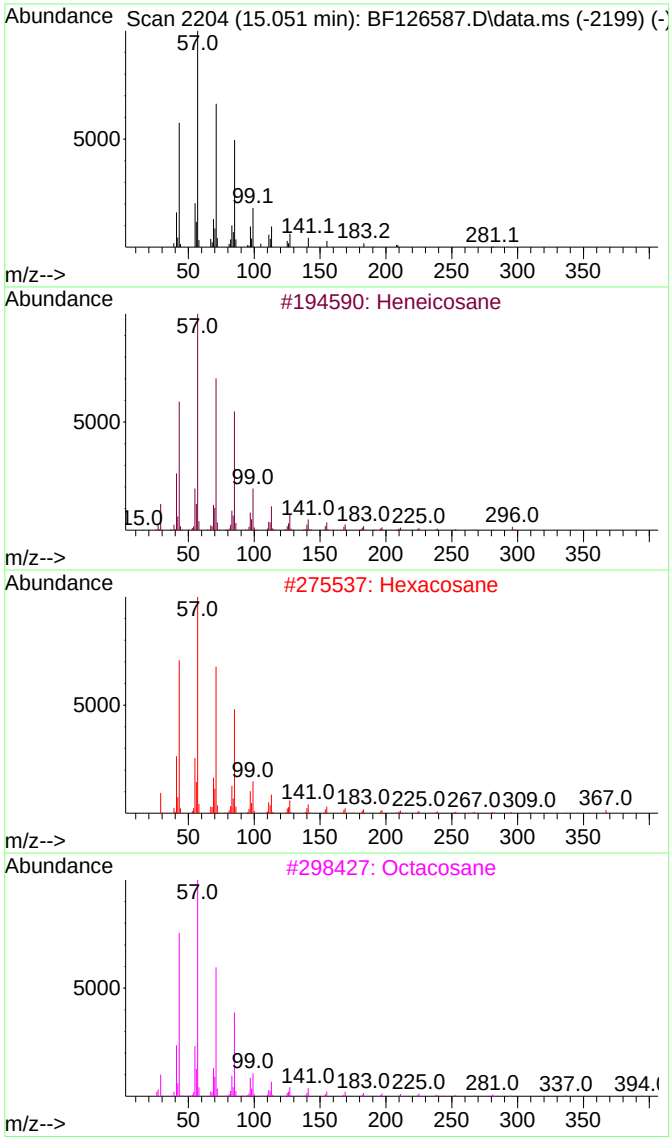
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

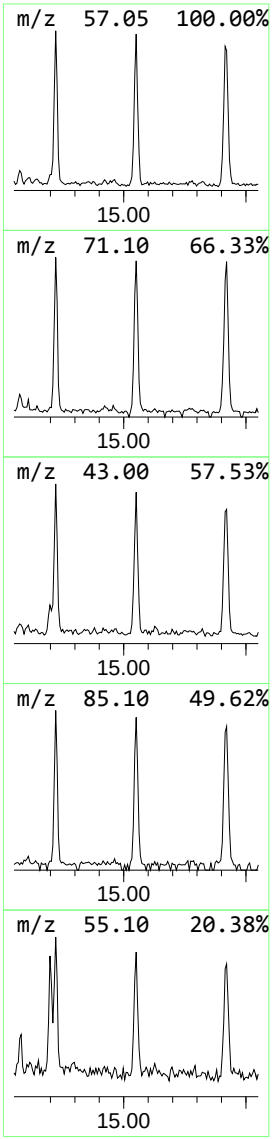
****

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	3.43 ng	99492	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

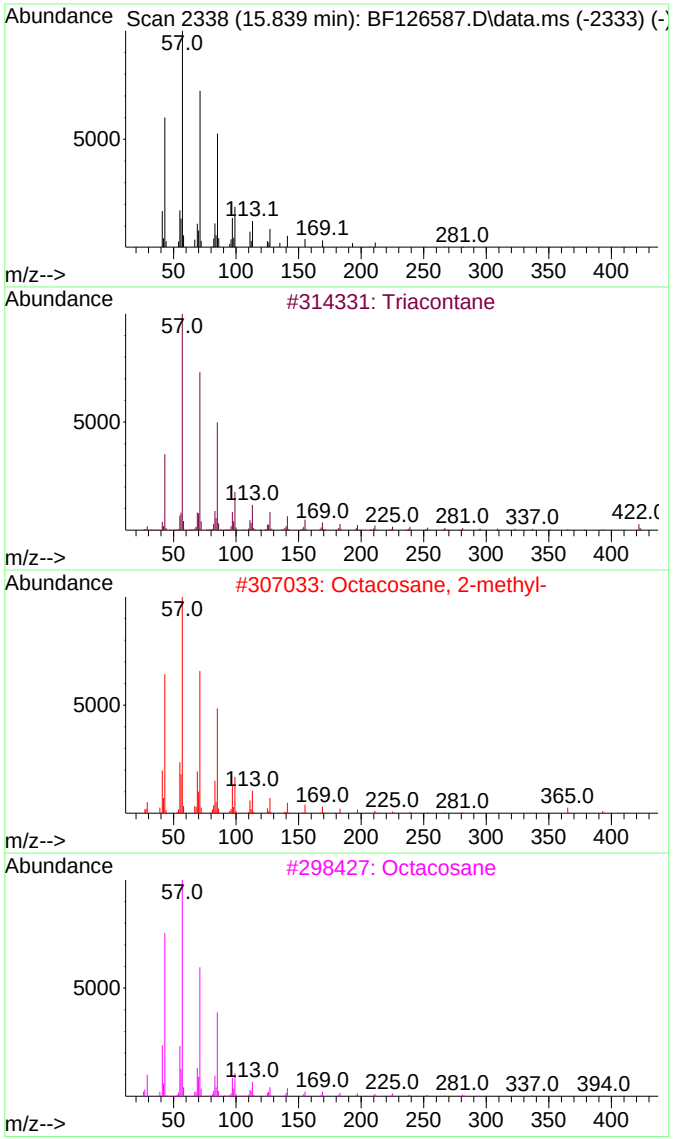
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

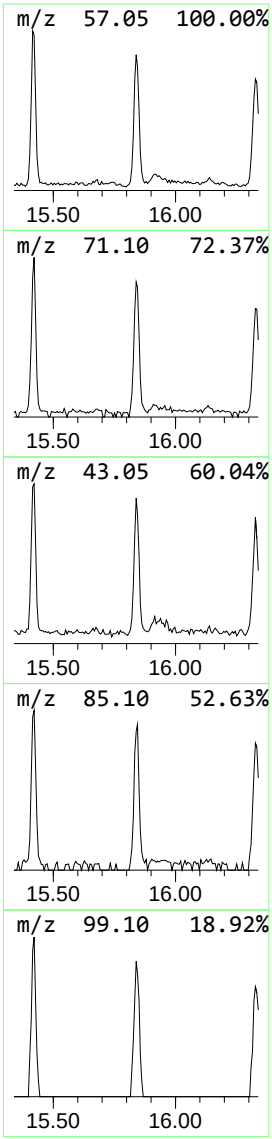
****

Peak Number 8 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	3.78 ng	109389	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heptadecane	240	C17H36	000629-78-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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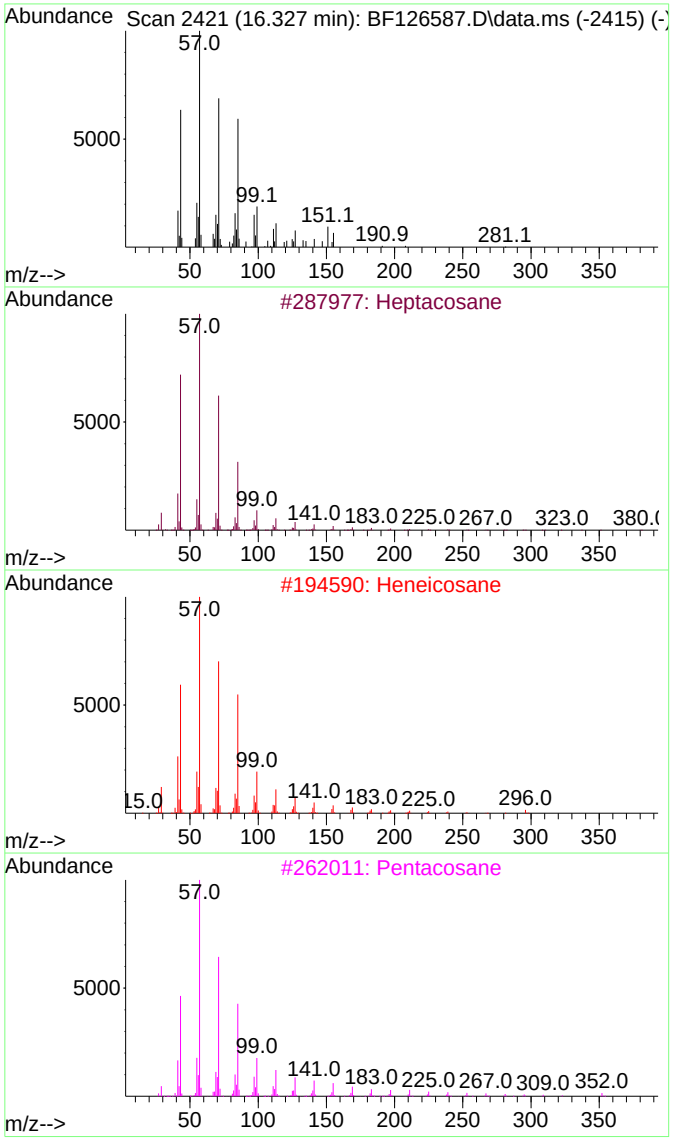
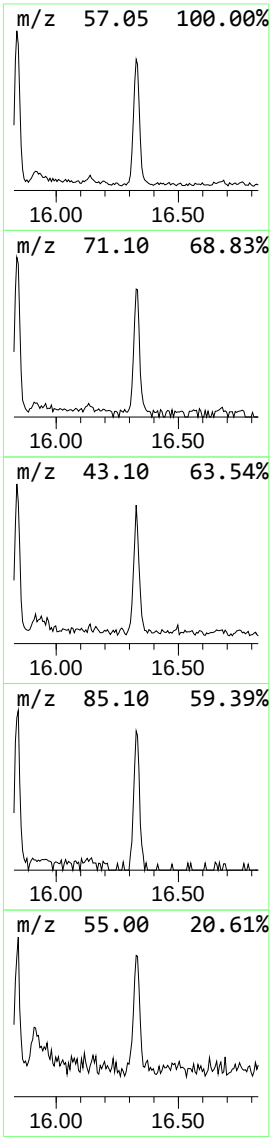
Peak Number 9 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	4.17 ng	120907	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	83
5	Octadecane	254	C18H38	000593-45-3	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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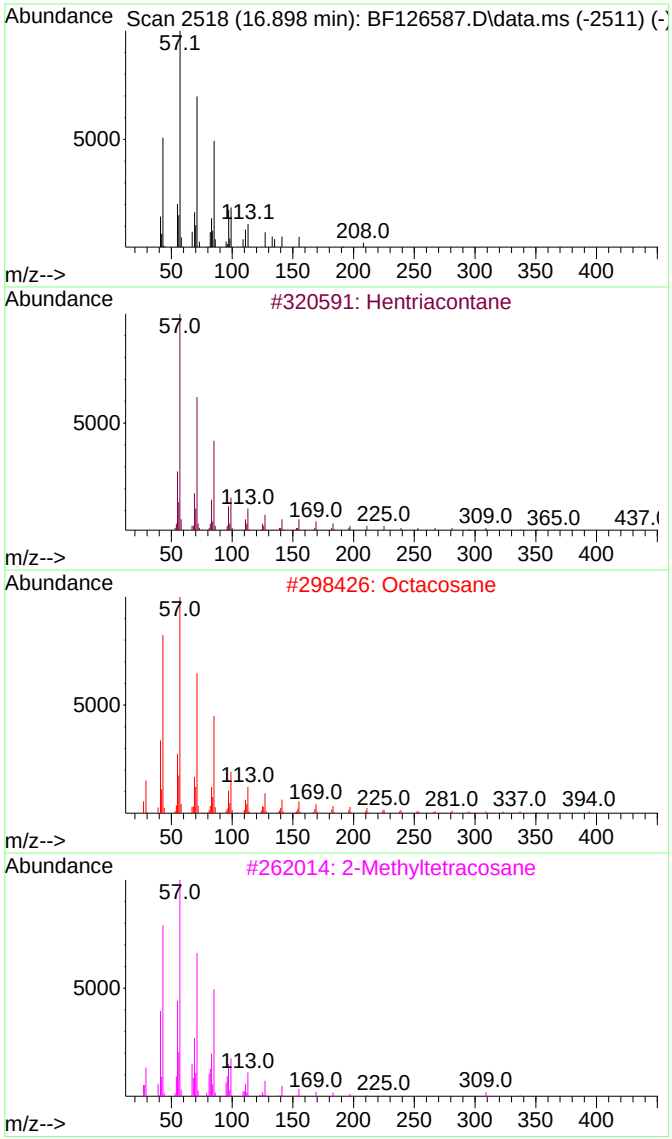
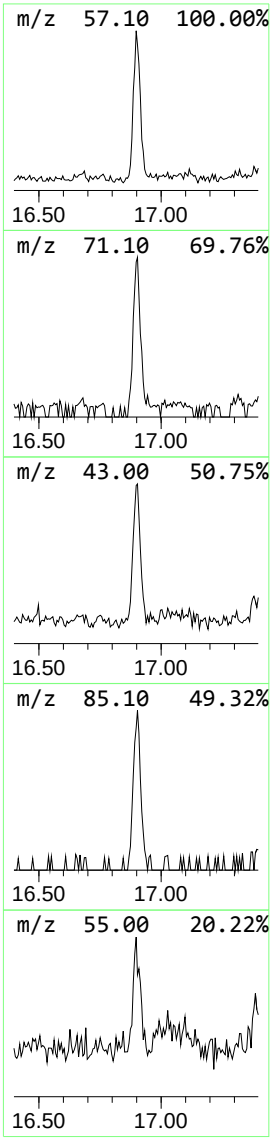
Peak Number 10 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	2.58 ng	74798	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-Methyltetracosane	352	C25H52	001560-78-7	90
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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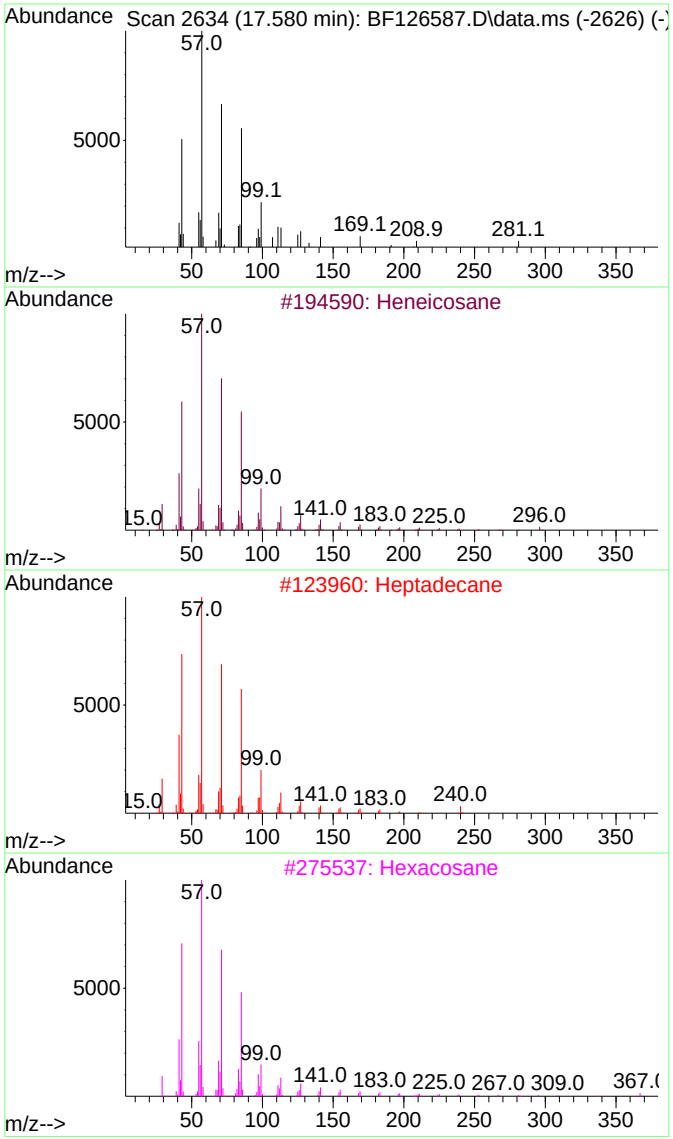
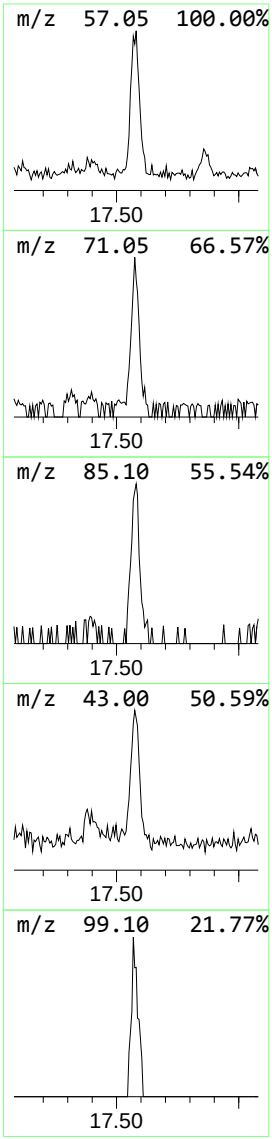
Peak Number 11 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.580	2.37 ng	68784	Perylene-d12	15.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Heptadecane	240	C17H36	000629-78-7	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	Octacosane	394	C28H58	000630-02-4	72
5	Pentacosane	352	C25H52	000629-99-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126587.D
Acq On : 11 Jan 2022 13:00
Operator : JU/CG
Sample : N1054-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	7.957	12.6	ng	485887	2	8.051	772387	20.0
n-Hexadecanoic ...	11.833	4.2	ng	167738	4	11.292	808327	20.0
1-Decanol, 2-he...	13.792	10.7	ng	359707	5	13.939	675560	20.0
Dodecane, 1-iodo-	14.110	2.4	ng	79965	5	13.939	675560	20.0
Heneicosane	14.421	2.5	ng	84122	5	13.939	675560	20.0
Hexacosane	14.721	2.8	ng	81434	6	15.380	579389	20.0
Octacosane	15.051	3.4	ng	99492	6	15.380	579389	20.0
Triacontane	15.839	3.8	ng	109389	6	15.380	579389	20.0
Heptacosane	16.327	4.2	ng	120907	6	15.380	579389	20.0
Hentriacontane	16.898	2.6	ng	74798	6	15.380	579389	20.0
Pentacosane	17.580	2.4	ng	68784	6	15.380	579389	20.0