LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137205.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	21	rVB2	13400	18001	1.21%	0.153%
2	5.016	490	498	506	rBV	132975	171199	11.48%	1.455%
3	5.422	563	567	576	rBV	1334428	1253425	84.06%	10.652%
4	6.422	732	737	754	rBV	1276105	1260316	84.52%	10.711%
5	6.793	796	800	809	rBV	344779	303036	20.32%	2.575%
6	7.351	890	895	905	rBV	851955	807162	54.13%	6.860%
7	8.069	1013	1017	1029	rBV	426083	398292	26.71%	3.385%
8	9.145	1196	1200	1203	rBV	1820617	1491120	100.00%	12.672%
9	9.822	1311	1315	1326	rVB	548197	441586	29.61%	3.753%
10	10.610	1446	1449	1460	rBV	953735	904899	60.69%	7.690%
11	11.198	1533	1549	1551	rBV3	13146	33054	2.22%	0.281%
12	11.316	1565	1569	1577	rBV	450710	435634	29.22%	3.702%
13	11.857	1658	1661	1675	rBV2	114942	183117	12.28%	1.556%
14	12.527	1771	1775	1779	rBV	25064	24183	1.62%	0.206%
15	12.610	1779	1789	1792	rBV3	51000	119433	8.01%	1.015%
16	12.651	1792	1796	1805	rVB3	78611	139263	9.34%	1.184%
17	12.757	1811	1814	1819	rVB	28445	27789	1.86%	0.236%
18	12.916	1836	1841	1844	rBV	1507839	1387670	93.06%	11.793%
19	13.016	1849	1858	1868	rVB	332180	668260	44.82%	5.679%
20	13.427	1920	1928	1933	rBV	62722	111990	7.51%	0.952%
21	13.545	1943	1948	1956	rVB6	9762	23734	1.59%	0.202%
22	13.833	1991	1997	2005	rBV	72991	116176	7.79%	0.987%
23	13.969	2016	2020	2027	rBV	380067	395288	26.51%	3.359%
24	14.039	2027	2032	2044	rVB	78448	138212	9.27%	1.175%
25	14.151	2048	2051	2054	rBV	18751	17329	1.16%	0.147%
26	14.463	2101	2104	2109	rBV	24749	27164	1.82%	0.231%
27	14.551	2115	2119	2126	rVB	76170	108214	7.26%	0.920%
28	14.751	2149	2153	2155	rBV4	17323	21883	1.47%	0.186%
29	14.774	2155	2157	2162	rVB2	26655	25834	1.73%	0.220%
30	15.074	2203	2208	2213	rBV	52547	87061	5.84%	0.740%
31	15.121	2213	2216	2220	rVB2	21713	26273	1.76%	0.223%
32	15.445	2266	2271	2279	rBV	299258	416150	27.91%	3.537%
33	15.521	2281	2284	2294	rVB5	13214	22340	1.50%	0.190%
34	15.668	2303	2309	2314	rBV2	36637	64108	4.30%	0.545%
35	16.345	2418	2424	2435	rVB5	16671	46399	3.11%	0.394%
36	17.139	2550	2559	2566	rBV4	18647	51396	3.45%	0.437%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

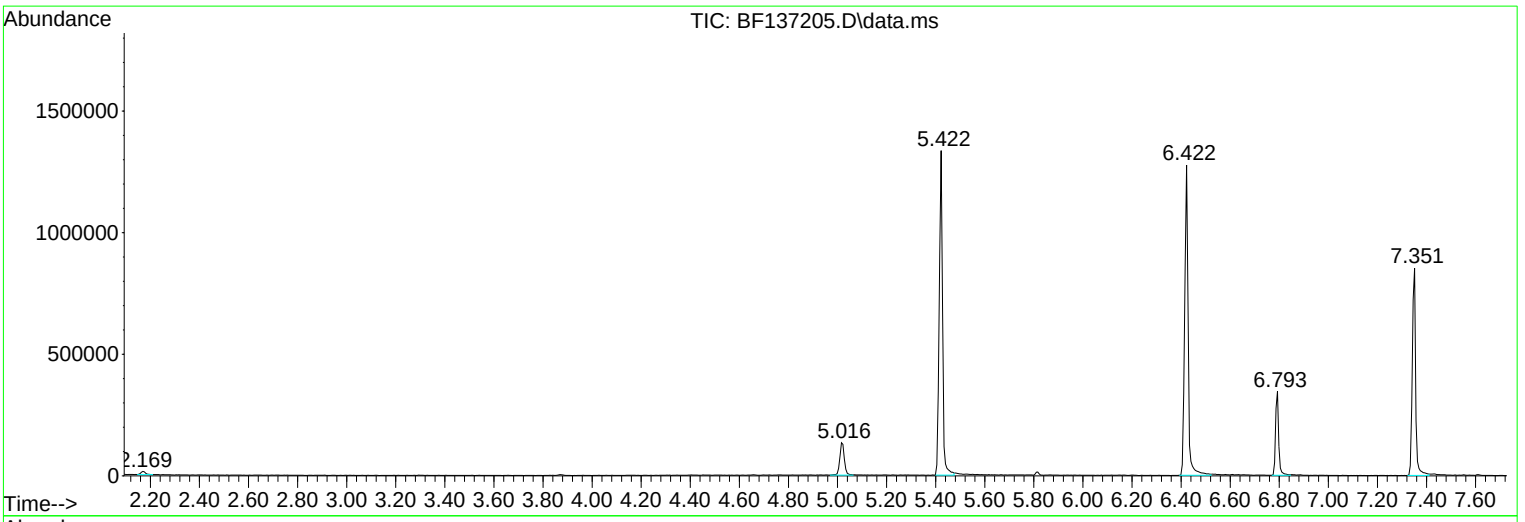
Sum of corrected areas: 11766990

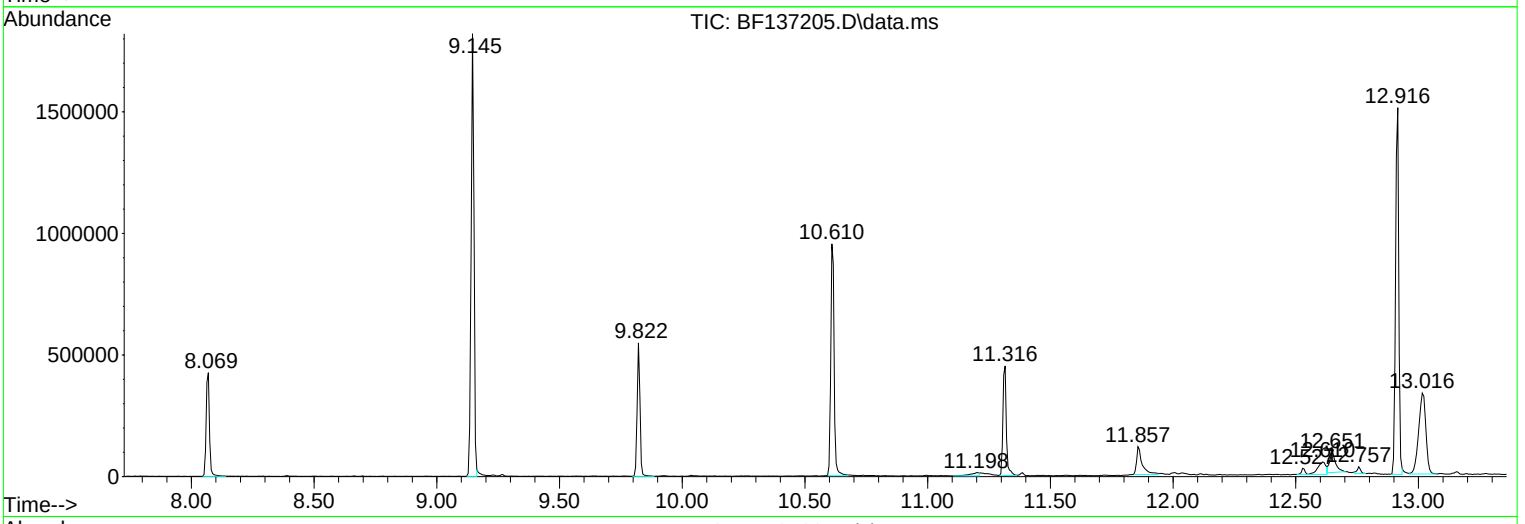
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

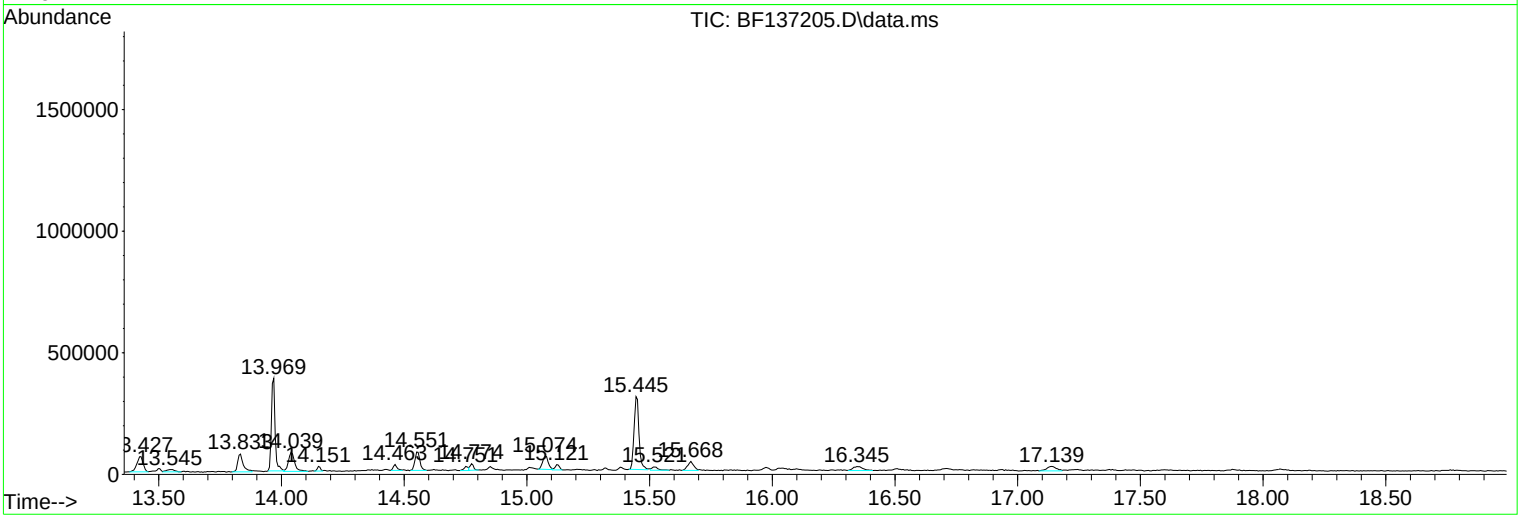
Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

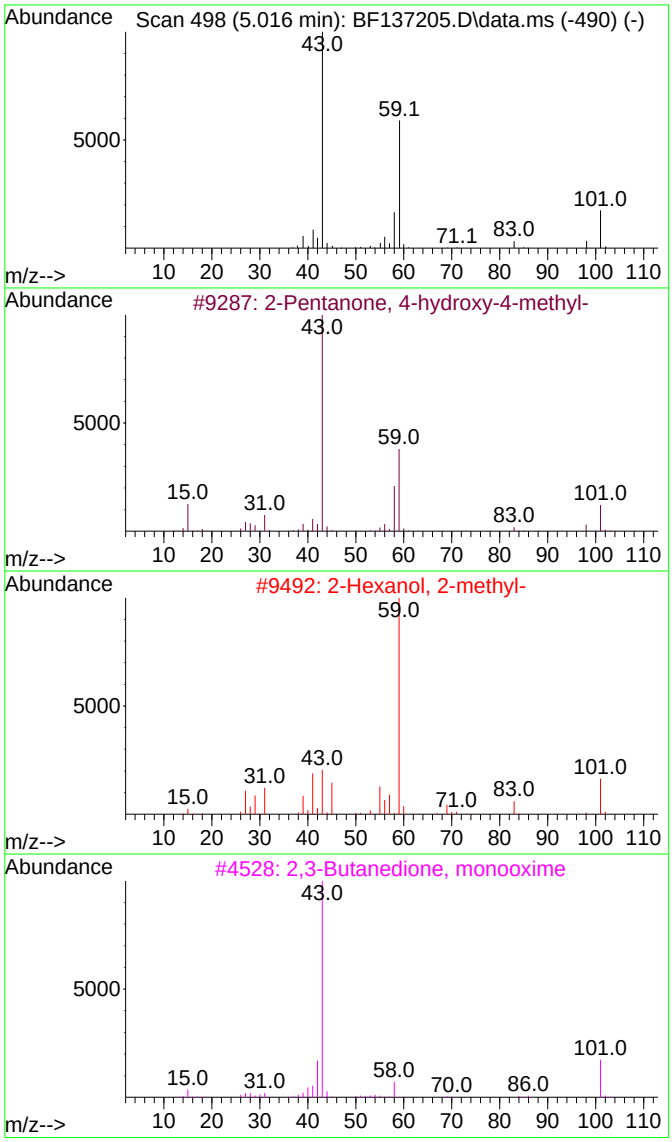
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

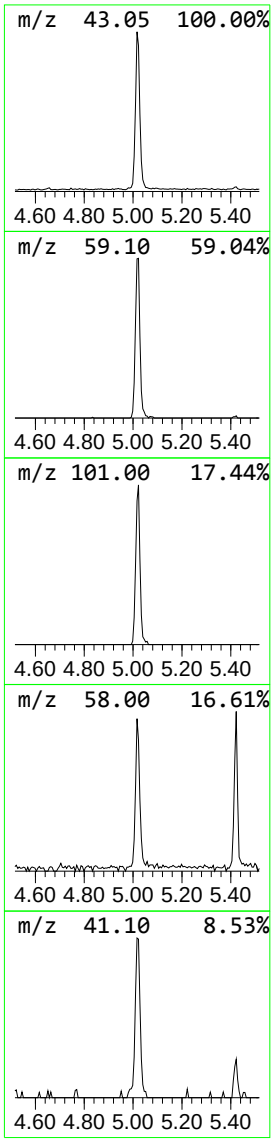
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	11.30 ng	171199	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

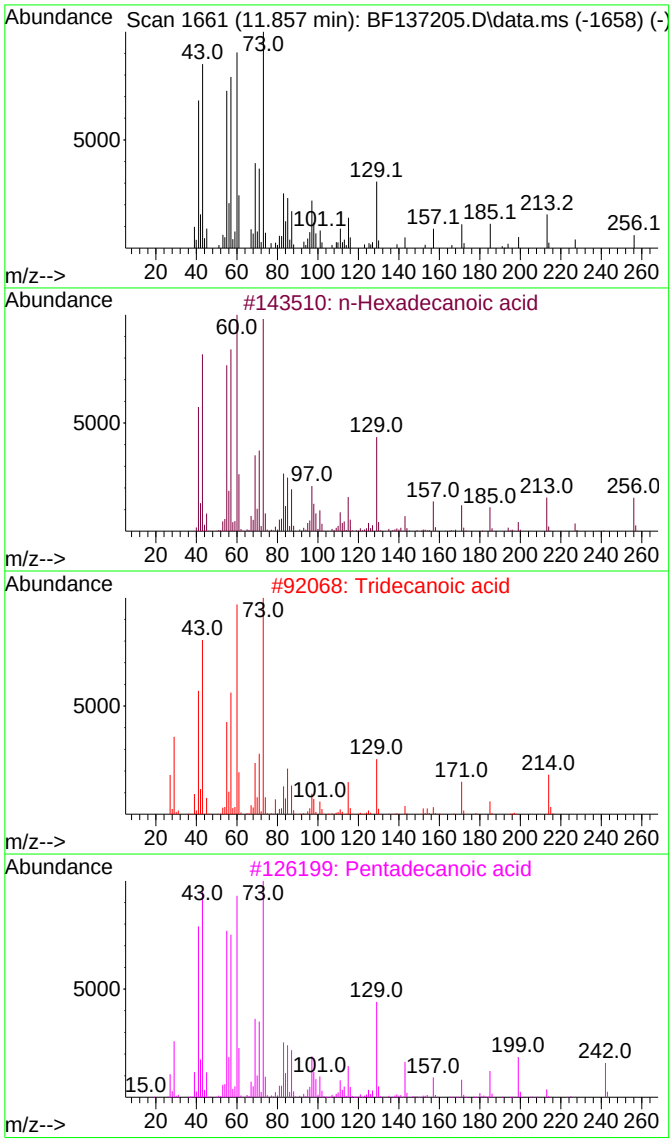
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

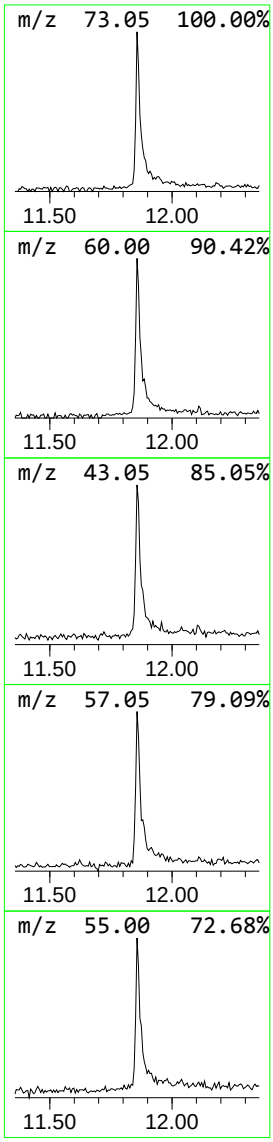
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.41 ng	183117	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

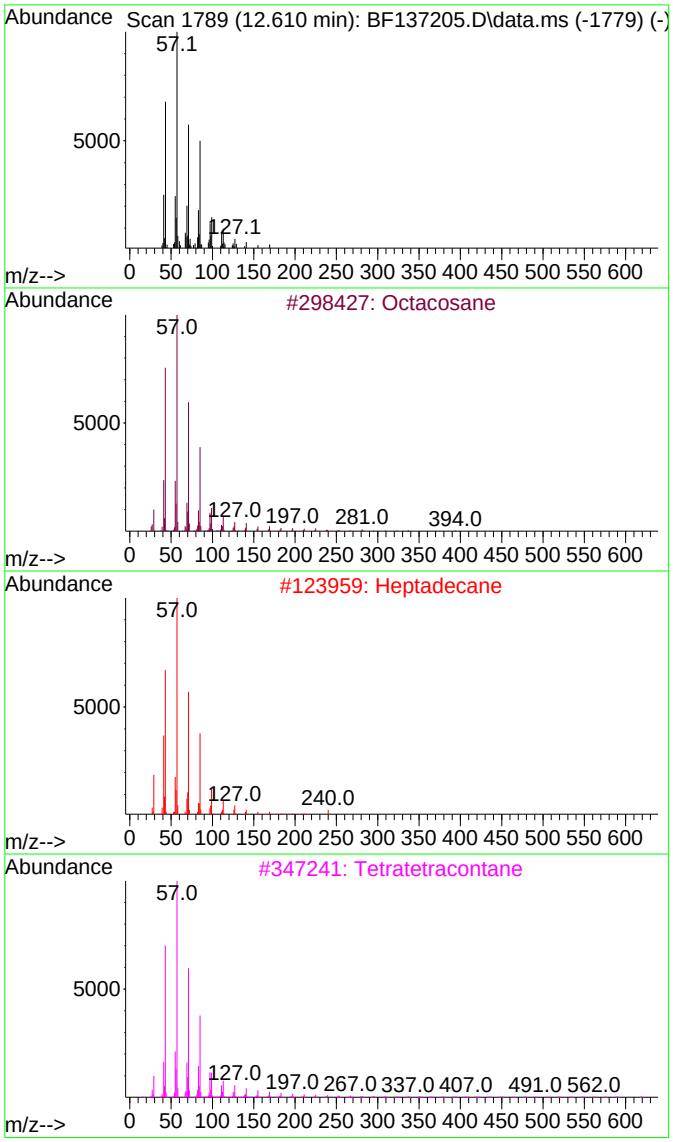
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

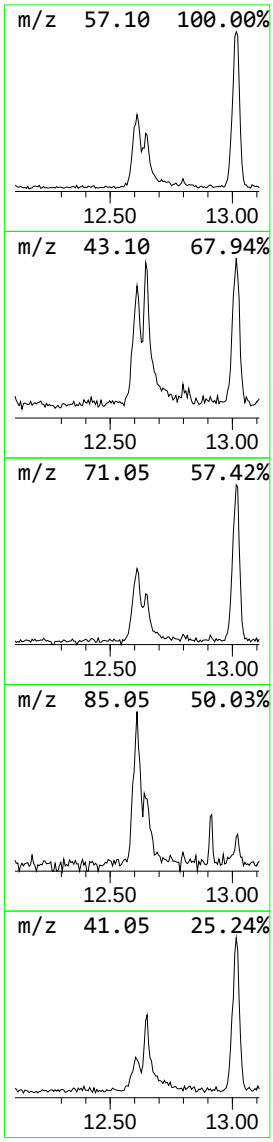
****

Peak Number 3 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	5.48 ng	119433	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Tetratetracontane	619	C44H90	007098-22-8	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Tritetracontane	605	C43H88	007098-21-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

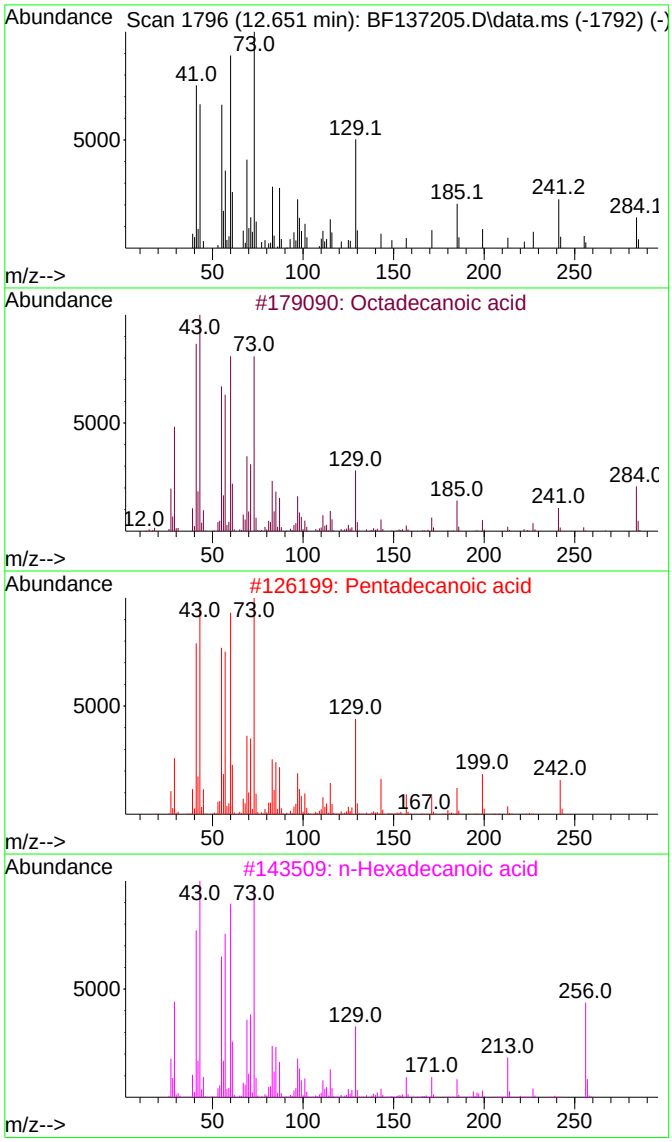
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

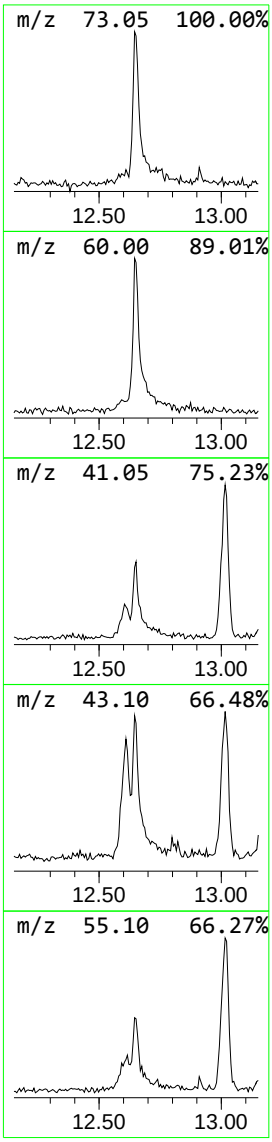
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	7.05 ng	139263	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

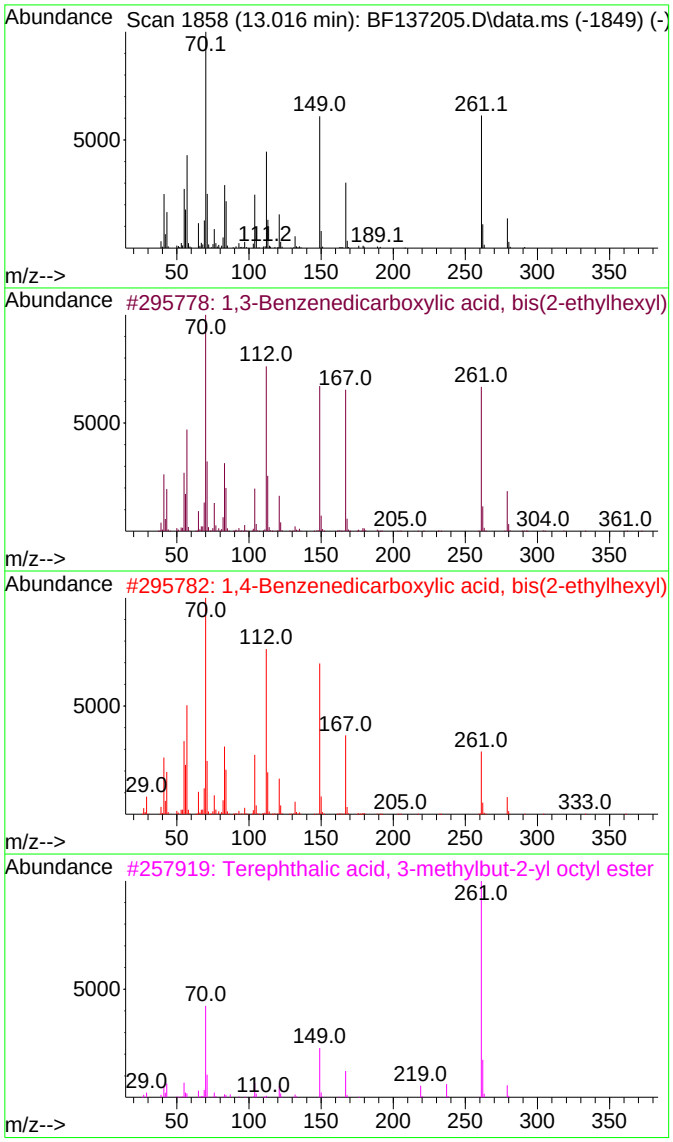
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

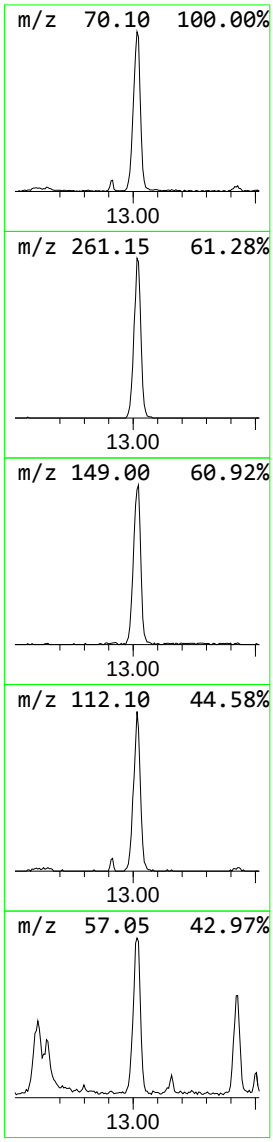
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.016	33.81 ng	668260	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
4	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	47
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	47





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Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

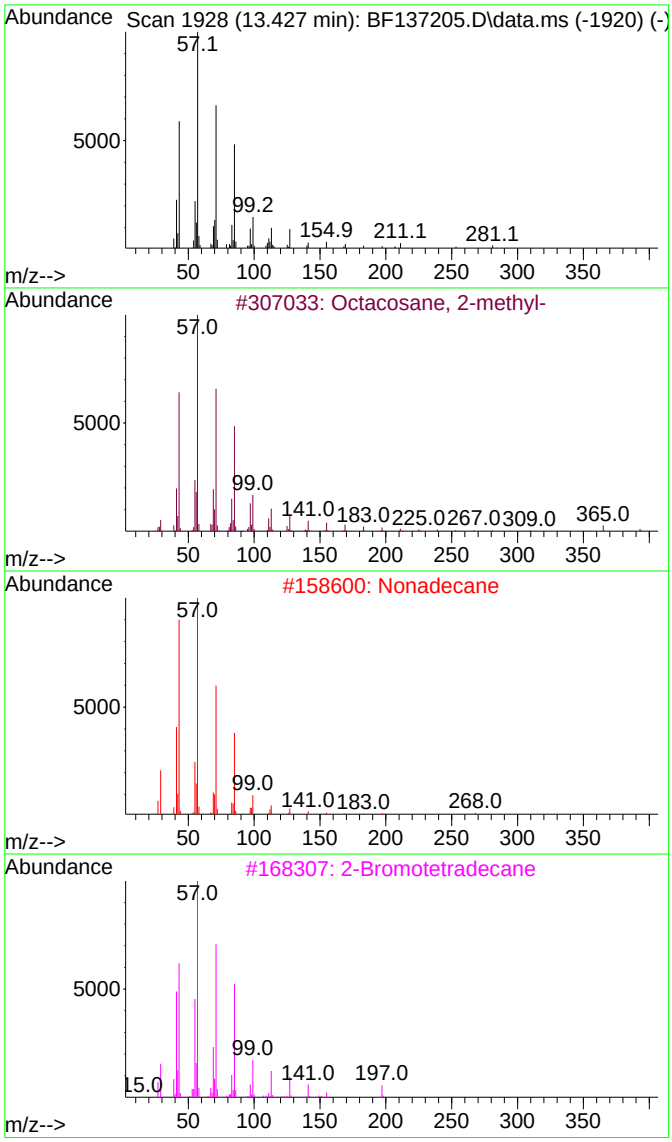
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

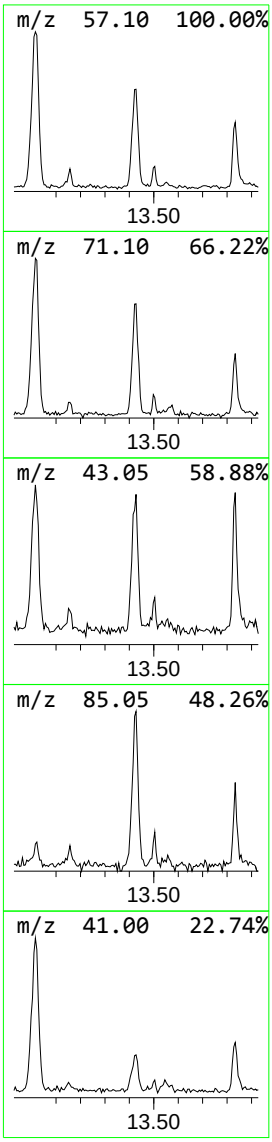
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	5.67 ng	111990	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

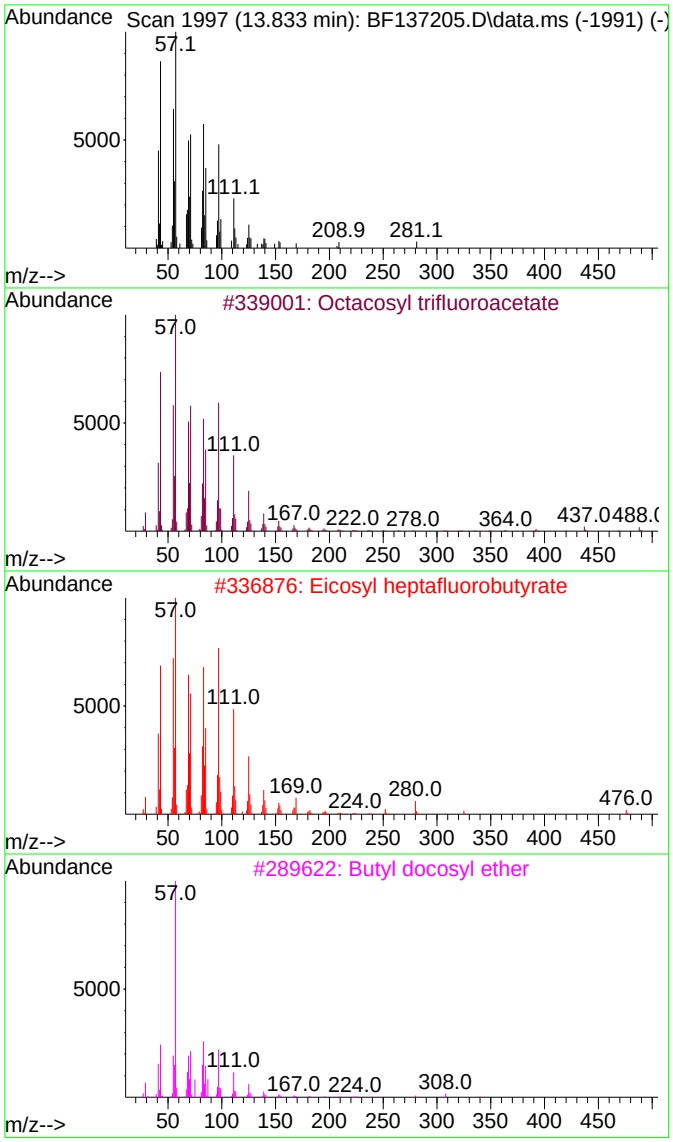
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

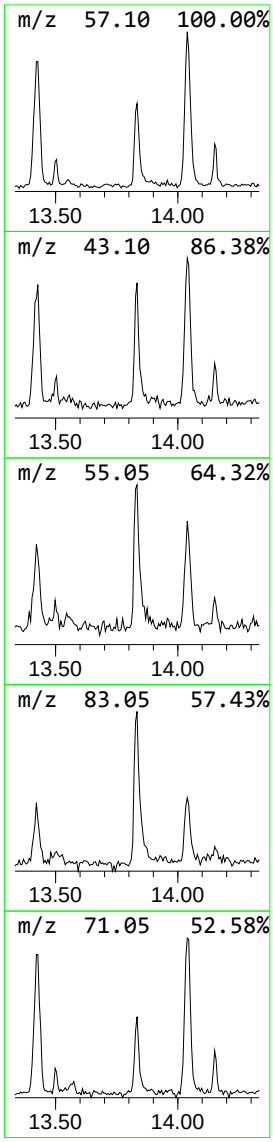
****

Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	5.88 ng	116176	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3	Butyl docosyl ether	382	C26H54O	1000406-40-8	91
4	Butyl hexacosyl ether	438	C30H62O	1000406-41-0	91
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

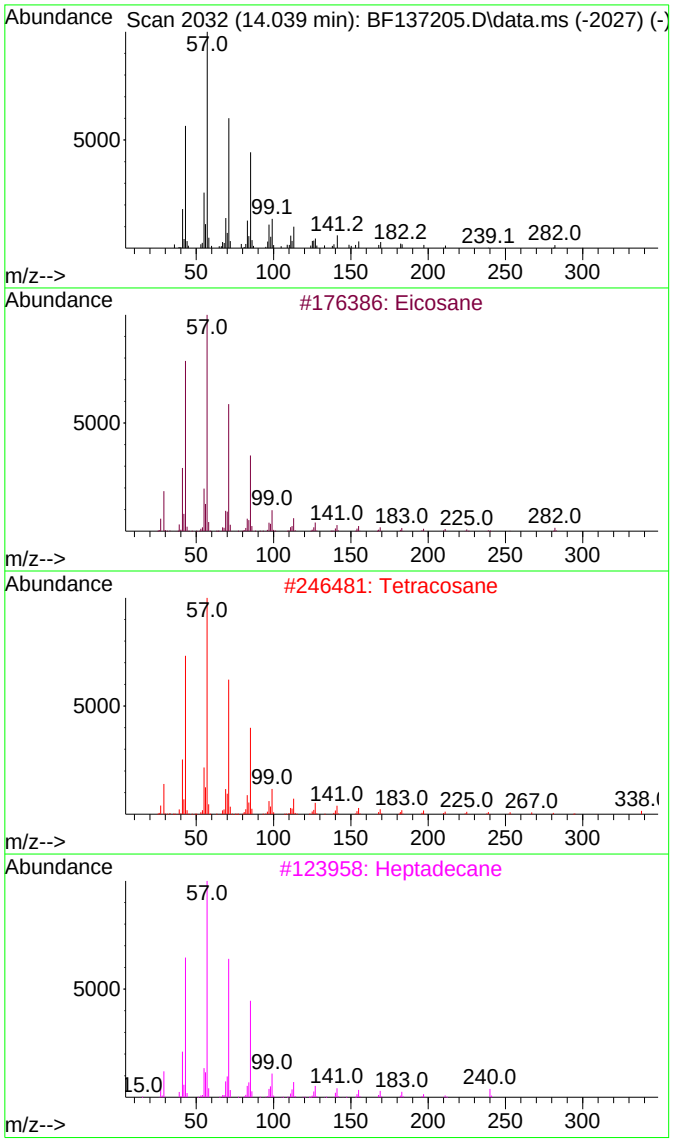
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

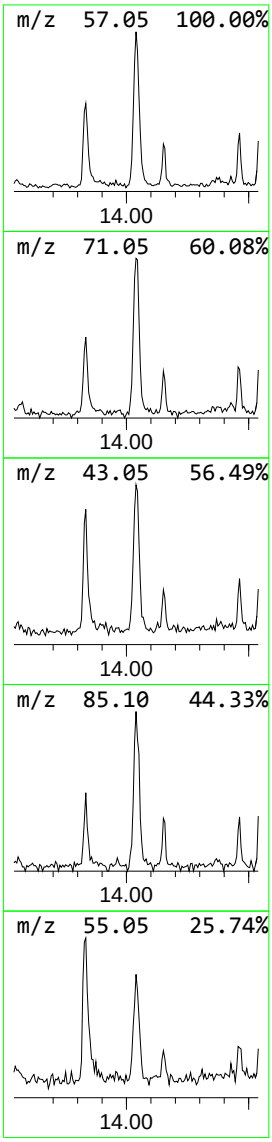
****

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	6.99 ng	138212	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
Data File : BF137205.D
Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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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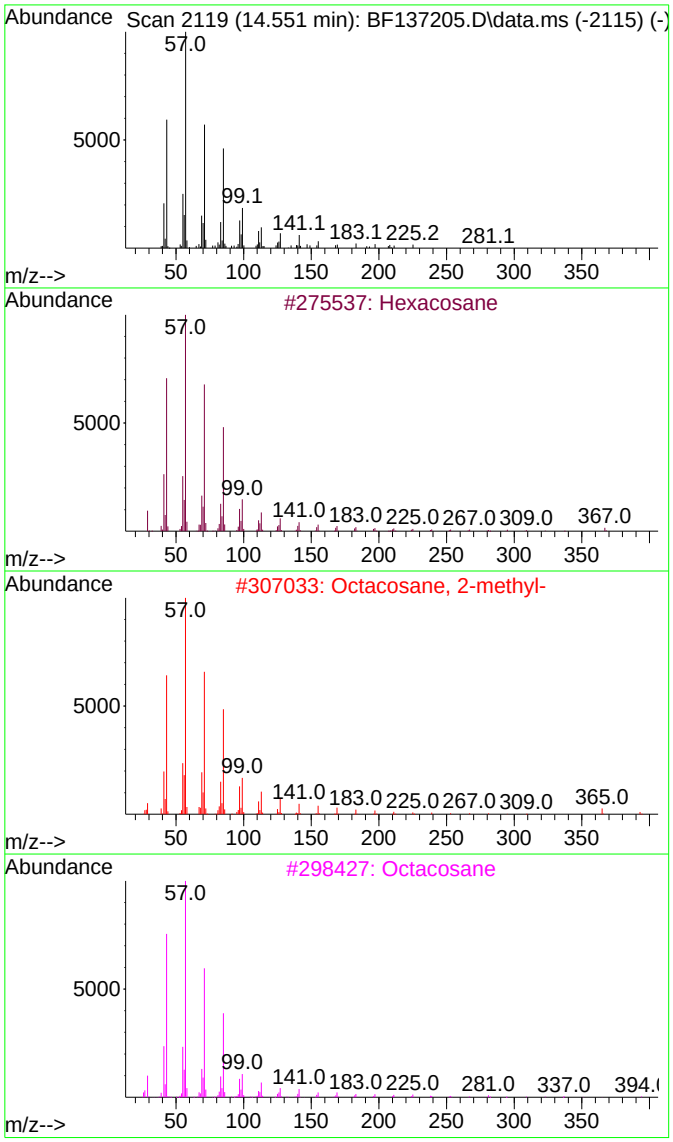
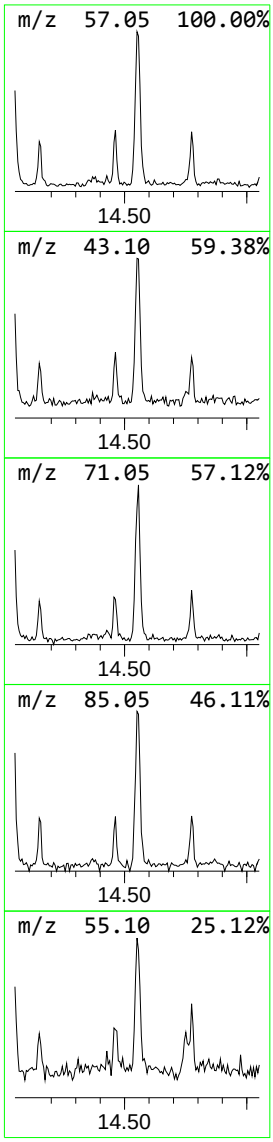
Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	5.48 ng	108214	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Pentacosane	352	C25H52	000629-99-2	90





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Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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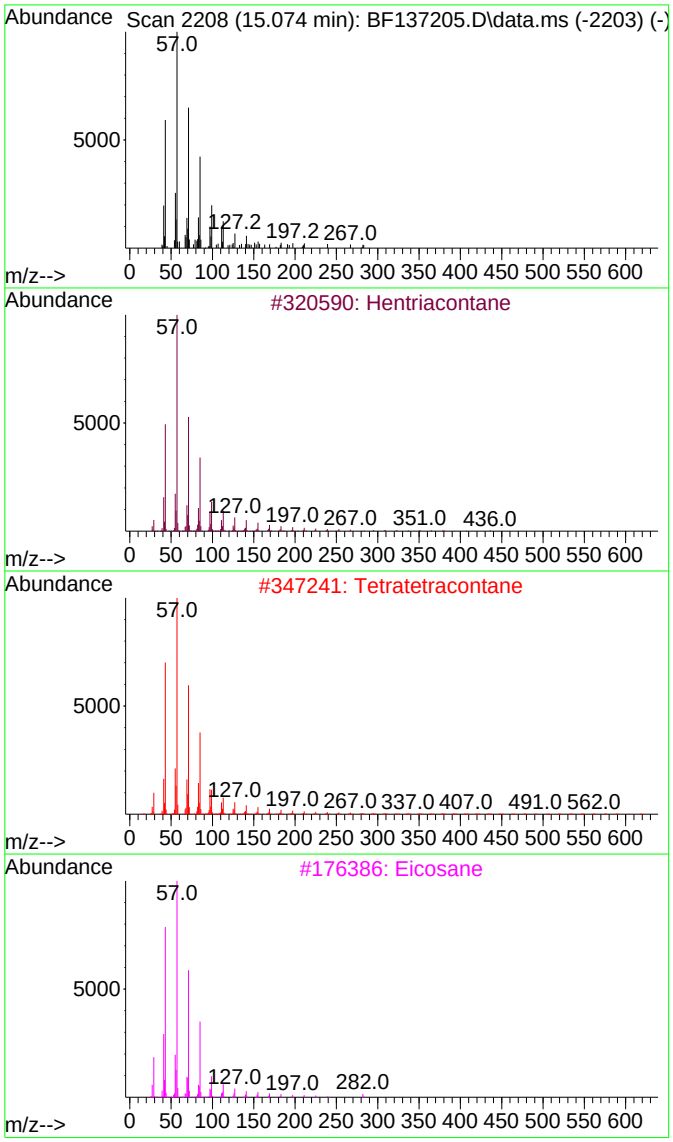
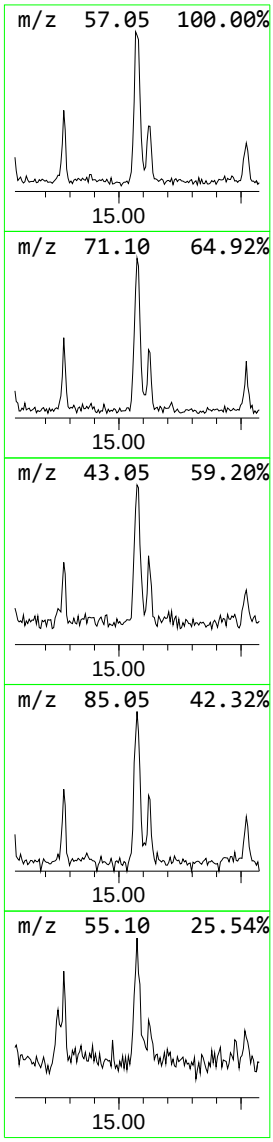
Peak Number 10 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	4.18 ng	87061	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Pentacosane	352	C25H52	000629-99-2	87





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Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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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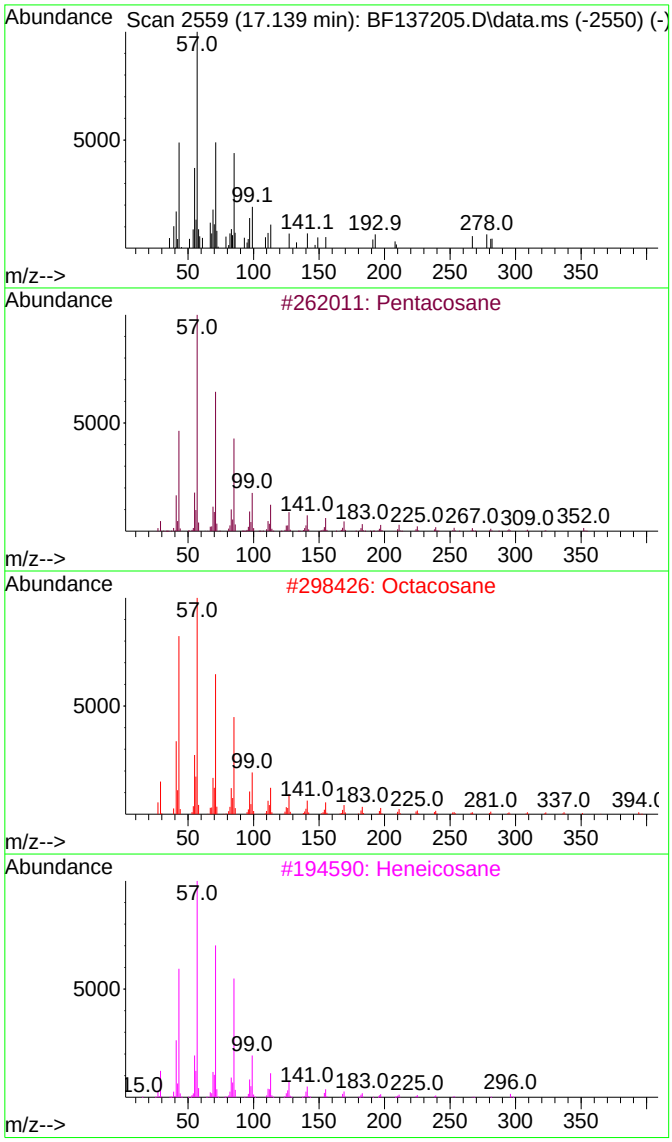
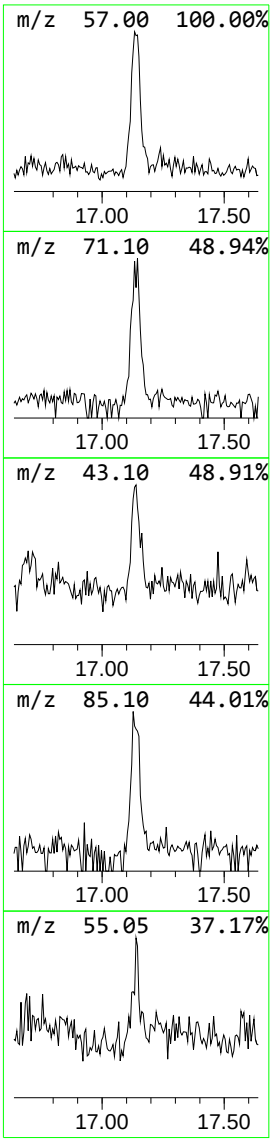
Peak Number 13 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	2.47 ng	51396	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Octacosane	394	C28H58	000630-02-4	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Eicosane	282	C20H42	000112-95-8	76
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF013124\
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Acq On : 31 Jan 2024 12:36
Operator : CG\JU
Sample : P1276-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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
2-Pentanone, 4-...	5.016	11.3	ng	171199	1	6.793	303036	20.0
n-Hexadecanoic ...	11.857	8.4	ng	183117	4	11.316	435634	20.0
Octacosane	12.610	5.5	ng	119433	4	11.316	435634	20.0
Octadecanoic acid	12.651	7.0	ng	139263	5	13.969	395288	20.0
1,3-Benzenedica...	13.016	33.8	ng	668260	5	13.969	395288	20.0
Octacosane, 2-m...	13.427	5.7	ng	111990	5	13.969	395288	20.0
Octacosyl trifl...	13.833	5.9	ng	116176	5	13.969	395288	20.0
Eicosane	14.039	7.0	ng	138212	5	13.969	395288	20.0
Hexacosane	14.551	5.5	ng	108214	5	13.969	395288	20.0
Hentriacontane	15.074	4.2	ng	87061	6	15.445	416150	20.0
Pentacosane	17.139	2.5	ng	51396	6	15.445	416150	20.0