LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GHL-SS-56

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136892.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	11	16	26	rVB2	17542	23969	1.31%	0.190%
2	5.028	496	500	507	rVB	30218	37123	2.03%	0.294%
3	5.428	564	568	582	rBV	1490998	1515207	82.90%	11.990%
4	6.428	734	738	741	rBV	1602072	1514897	82.88%	11.987%
5	6.781	794	798	801	rBV	532689	418595	22.90%	3.312%
6	7.345	889	894	897	rBV	1100656	1025924	56.13%	8.118%
7	8.057	1011	1015	1018	rBV	651230	536273	29.34%	4.243%
8	9.133	1193	1198	1201	rBV	2252080	1827828	100.00%	14.463%
9	9.180	1204	1206	1209	rVB	62658	52357	2.86%	0.414%
10	9.245	1214	1217	1221	rVB3	49486	43616	2.39%	0.345%
11	9.810	1309	1313	1316	rBV	664992	583343	31.91%	4.616%
12	9.833	1316	1317	1324	rVB3	33182	32719	1.79%	0.259%
13	10.604	1444	1448	1461	rVB	1126007	1036253	56.69%	8.200%
14	10.727	1465	1469	1472	rBV2	22609	32375	1.77%	0.256%
15	10.763	1472	1475	1479	rVB	30174	23211	1.27%	0.184%
16	11.304	1563	1567	1570	rBV	724219	571445	31.26%	4.522%
17	11.839	1654	1658	1668	rBV	244350	253749	13.88%	2.008%
18	11.921	1669	1672	1678	rVV4	56572	54564	2.99%	0.432%
19	11.992	1681	1684	1690	rVB3	23663	31653	1.73%	0.250%
20	12.551	1773	1779	1788	rBV6	35316	95497	5.22%	0.756%
21	12.627	1789	1792	1804	rVB2	58434	79088	4.33%	0.626%
22	12.898	1834	1838	1842	rBV	1572926	1463515	80.07%	11.581%
23	13.804	1989	1992	1995	rBV	24823	21857	1.20%	0.173%
24	13.857	1995	2001	2012	rVV7	24824	83583	4.57%	0.661%
25	13.957	2015	2018	2025	rVB	410877	375476	20.54%	2.971%
26	14.433	2095	2099	2103	rBV	41091	42864	2.35%	0.339%
27	14.739	2145	2151	2156	rVB3	19733	25005	1.37%	0.198%
28	14.815	2159	2164	2170	rBV	89902	98805	5.41%	0.782%
29	14.886	2173	2176	2179	rVB3	25951	24960	1.37%	0.198%
30	15.080	2206	2209	2213	rVB	42348	45582	2.49%	0.361%
31	15.439	2265	2270	2285	rVB	305664	417458	22.84%	3.303%
32	15.674	2306	2310	2315	rVB2	42328	56705	3.10%	0.449%
33	15.915	2347	2351	2356	rVB3	27683	36730	2.01%	0.291%
34	16.468	2443	2445	2453	rVB2	11624	22730	1.24%	0.180%
35	16.733	2486	2490	2499	rVB7	25295	47250	2.59%	0.374%
36	16.986	2527	2533	2540	rVB5	28088	54503	2.98%	0.431%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.580	2796	2804	2814	rBV5	10796	30867	1.69%	0.244%

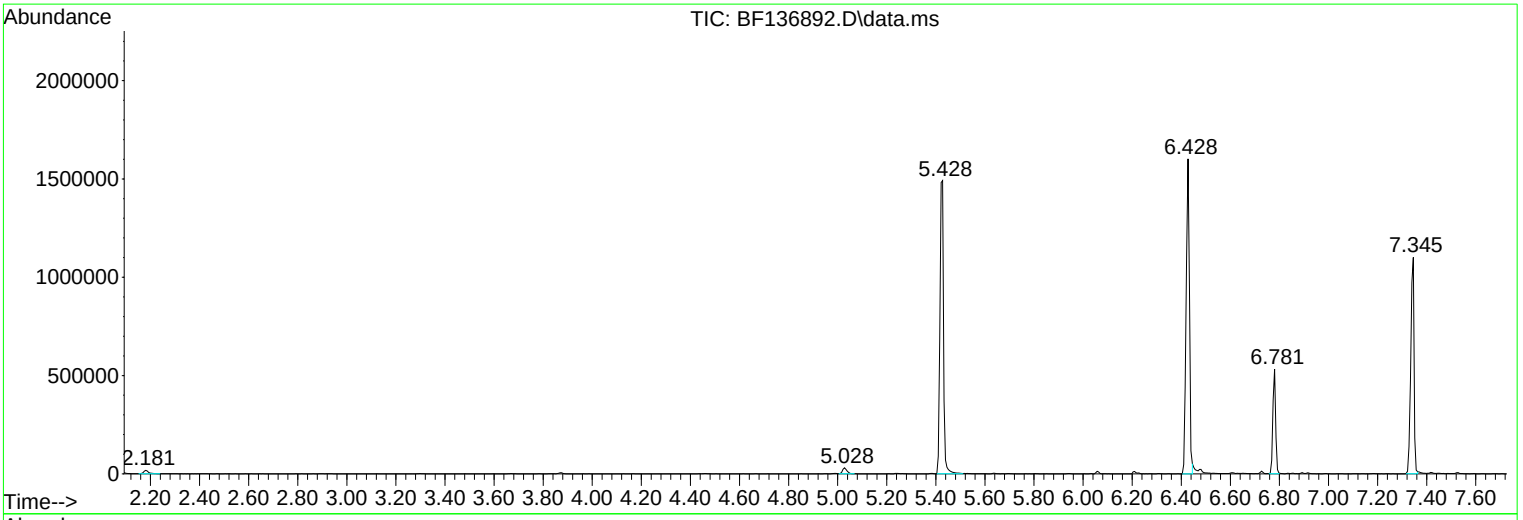
Sum of corrected areas: 12637576

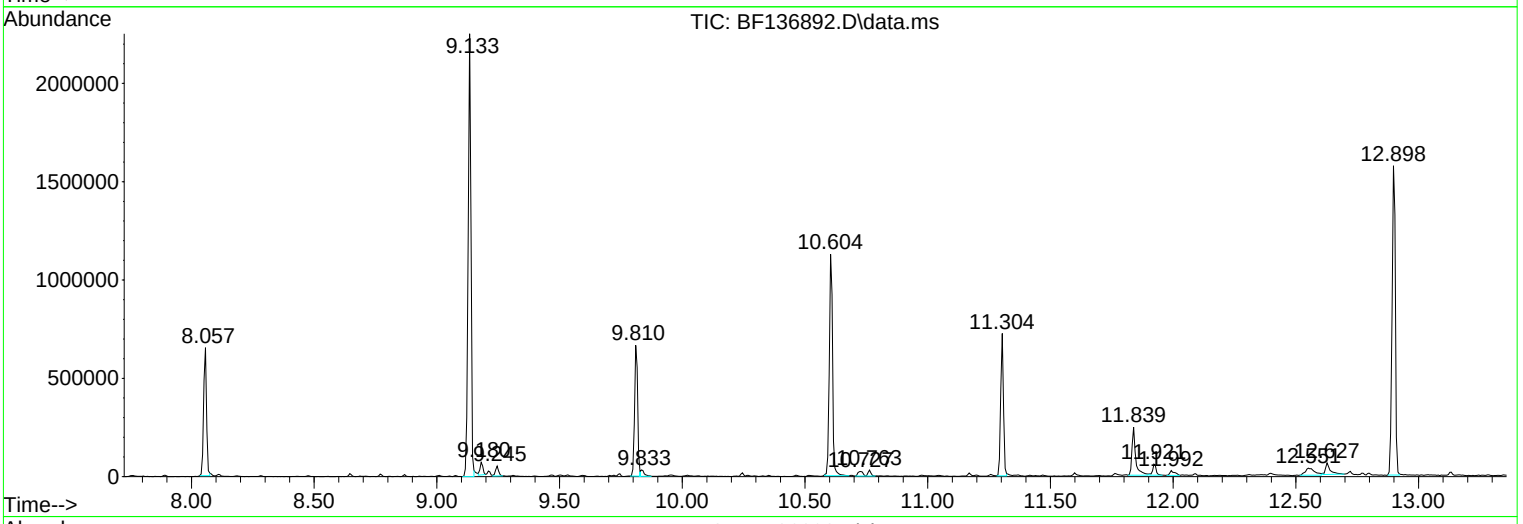
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

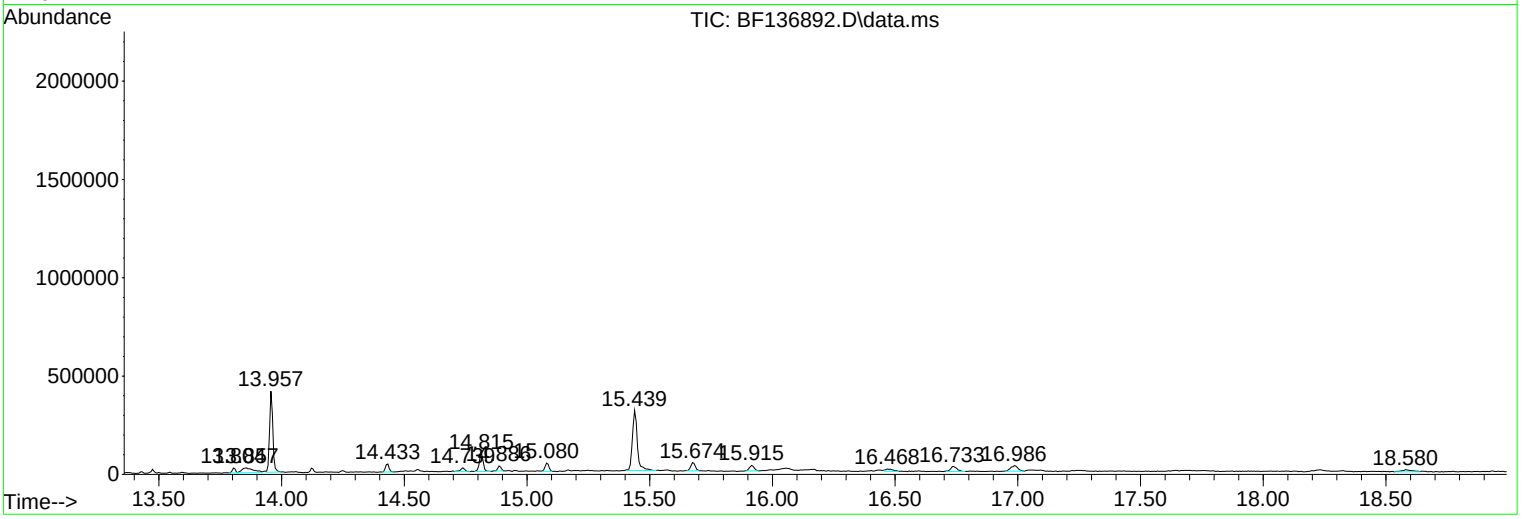
Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

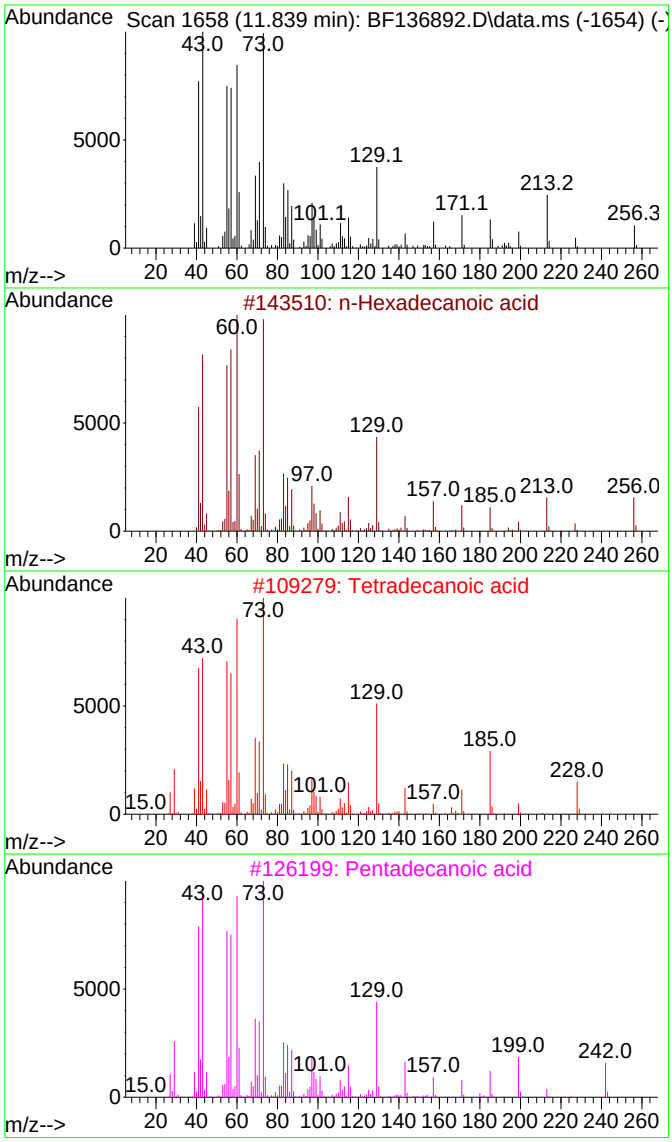
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

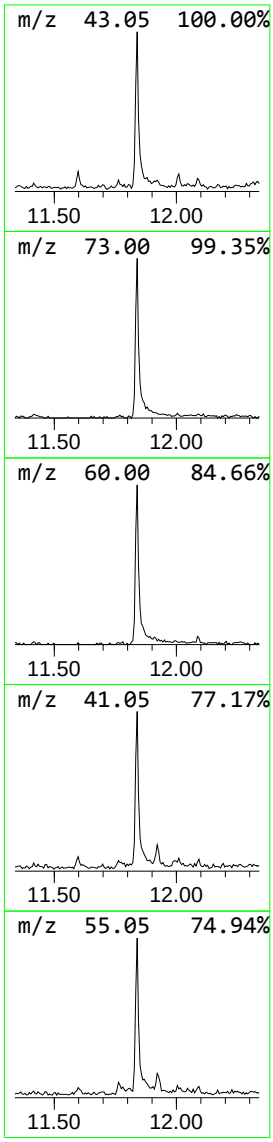
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	8.88 ng	253749	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

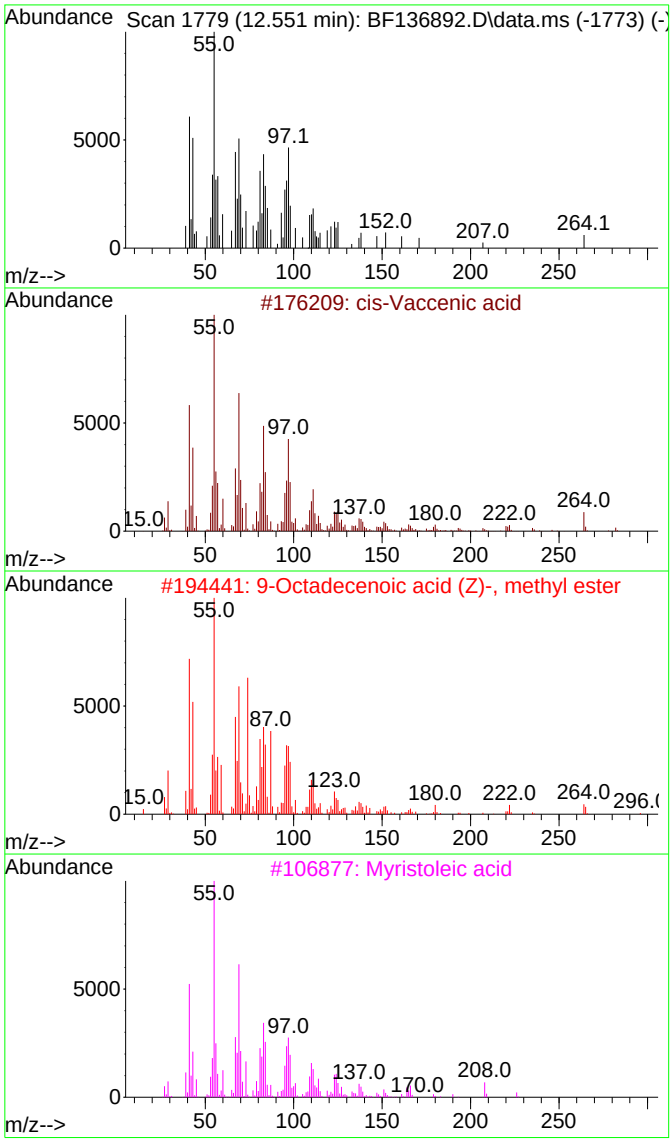
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

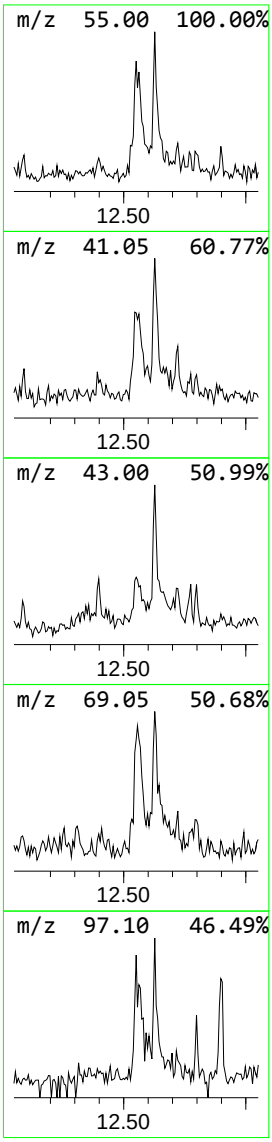
****

Peak Number 2 cis-Vaccenic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	3.34 ng	95497	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	72
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	64
3	Myristoleic acid	226	C14H26O2	000544-64-9	58
4	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	52
5	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

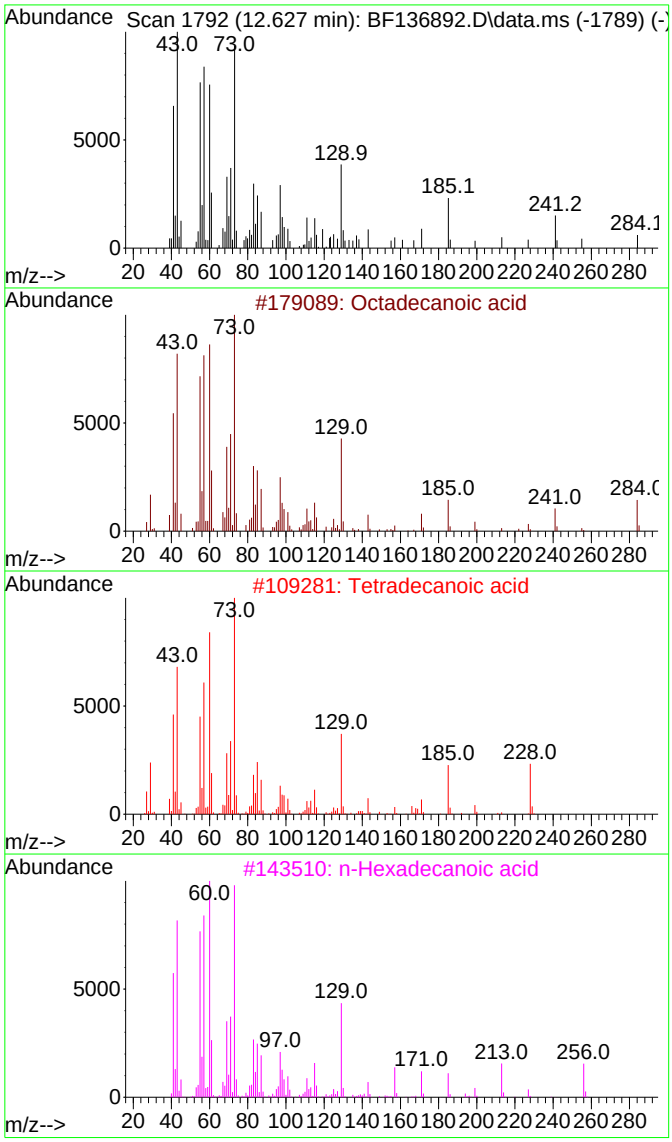
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

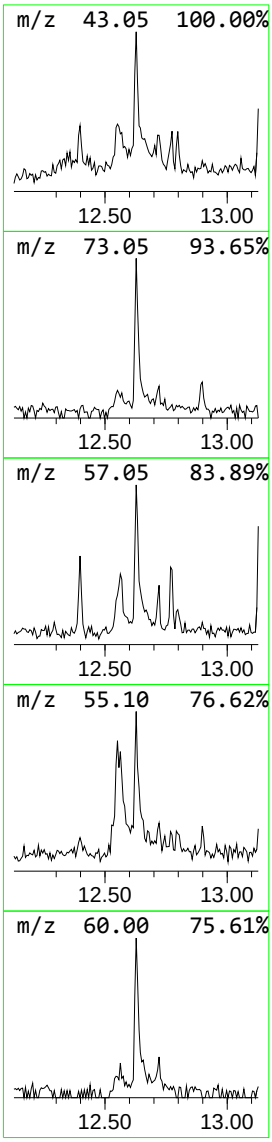
****

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.77 ng	79088	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

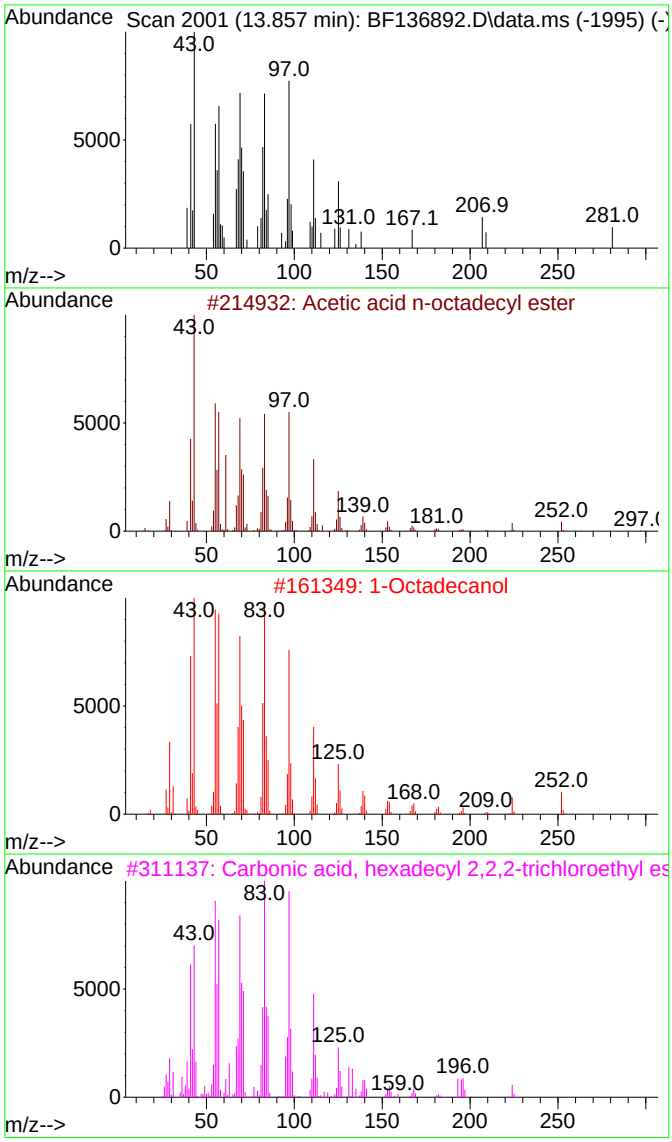
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

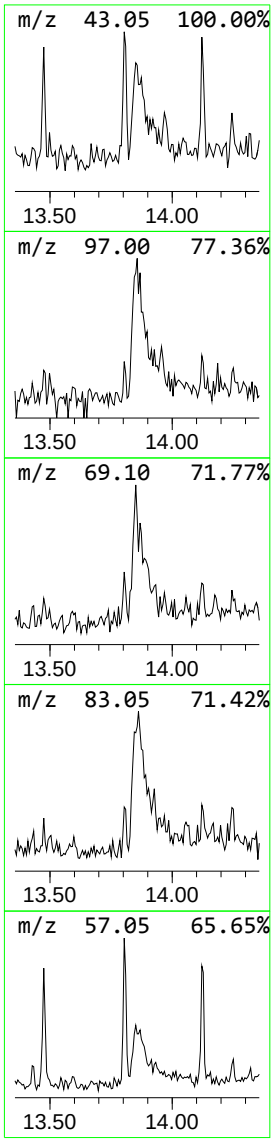
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetic acid n-octadecyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.45 ng	83583	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	91
2	1-Octadecanol	270	C18H38O	000112-92-5	87
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	86
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

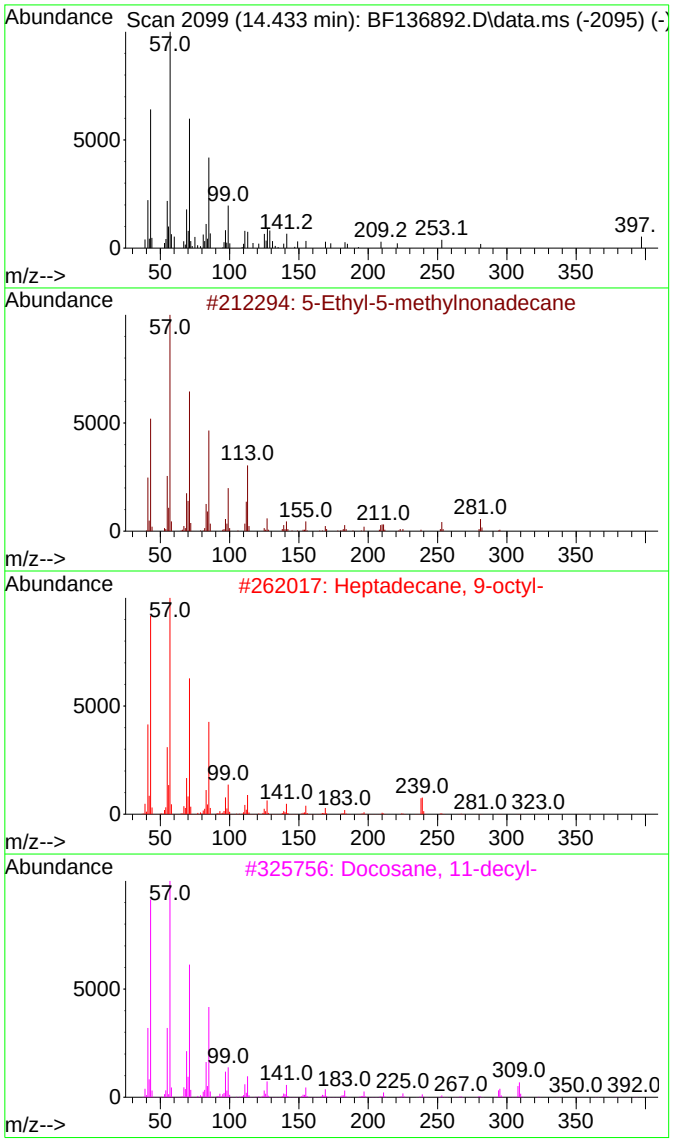
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

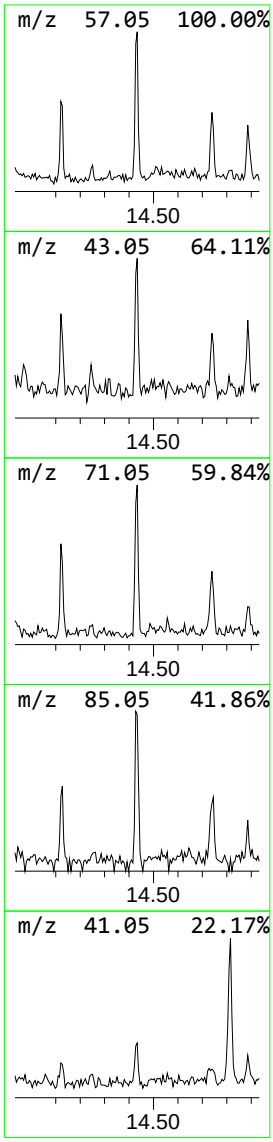
****

Peak Number 5 5-Ethyl-5-methylnonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.28 ng	42864	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	74
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	72
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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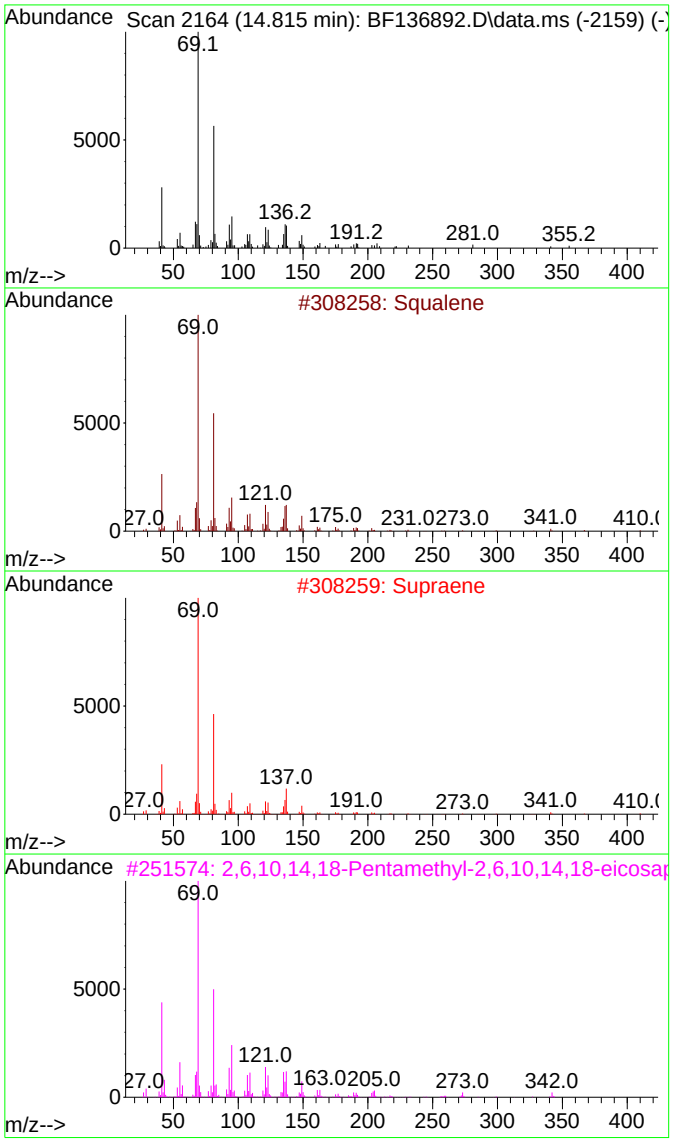
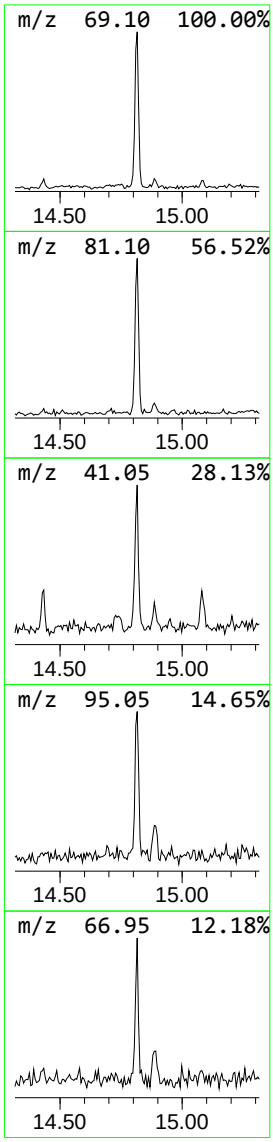
Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	4.73 ng	98805	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
5	Farnesol isomer a	222	C15H26O	1000108-92-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
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Operator : CG\JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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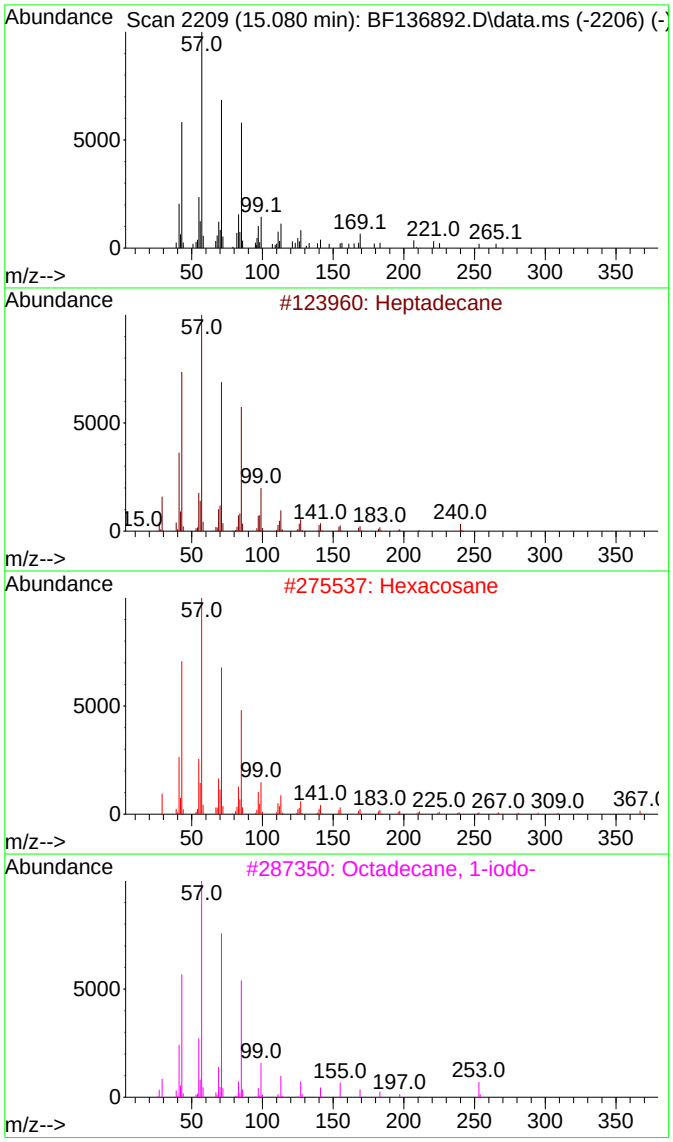
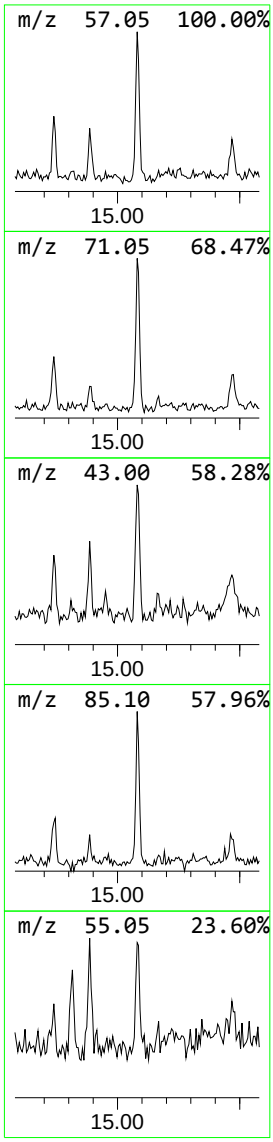
Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.18 ng	45582	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Hexacosane	366	C26H54	000630-01-3	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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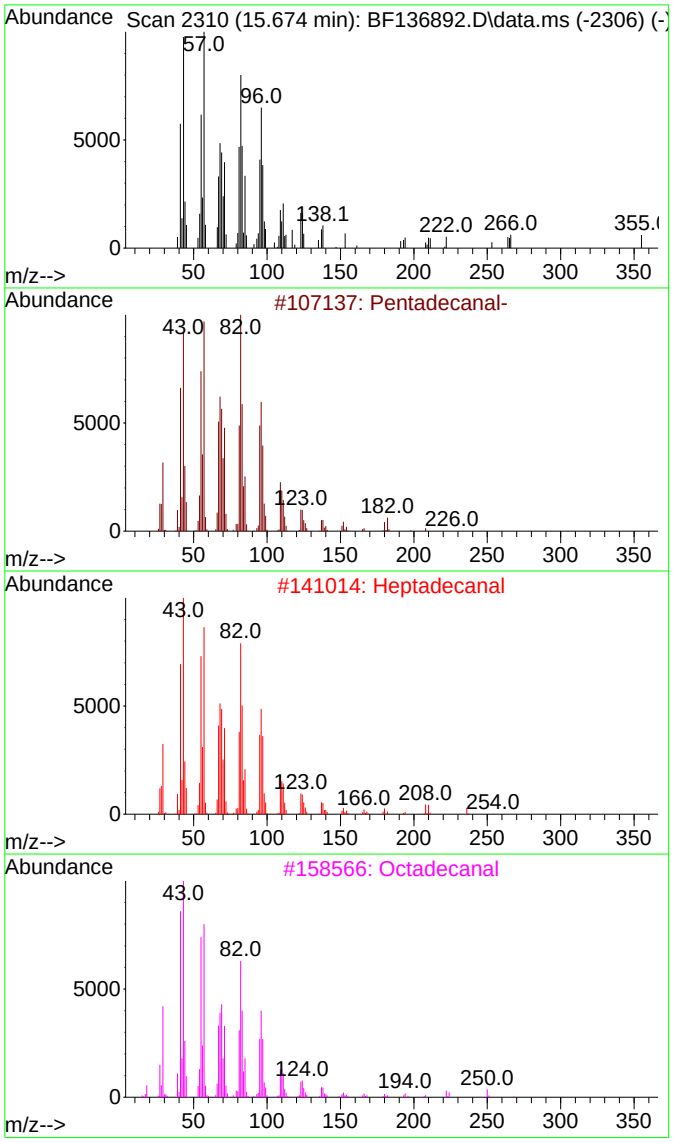
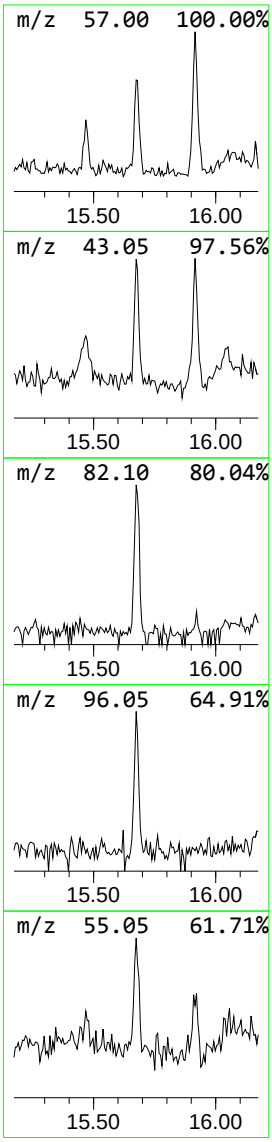
Peak Number 8 Pentadecanal- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.674	2.72 ng	56705	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-	226	C15H30O	002765-11-9	87
2	Heptadecanal	254	C17H34O	1000376-70-0	87
3	Octadecanal	268	C18H36O	000638-66-4	86
4	16-Octadecenal	266	C18H34O	056554-87-1	86
5	Hexadecanal	240	C16H32O	000629-80-1	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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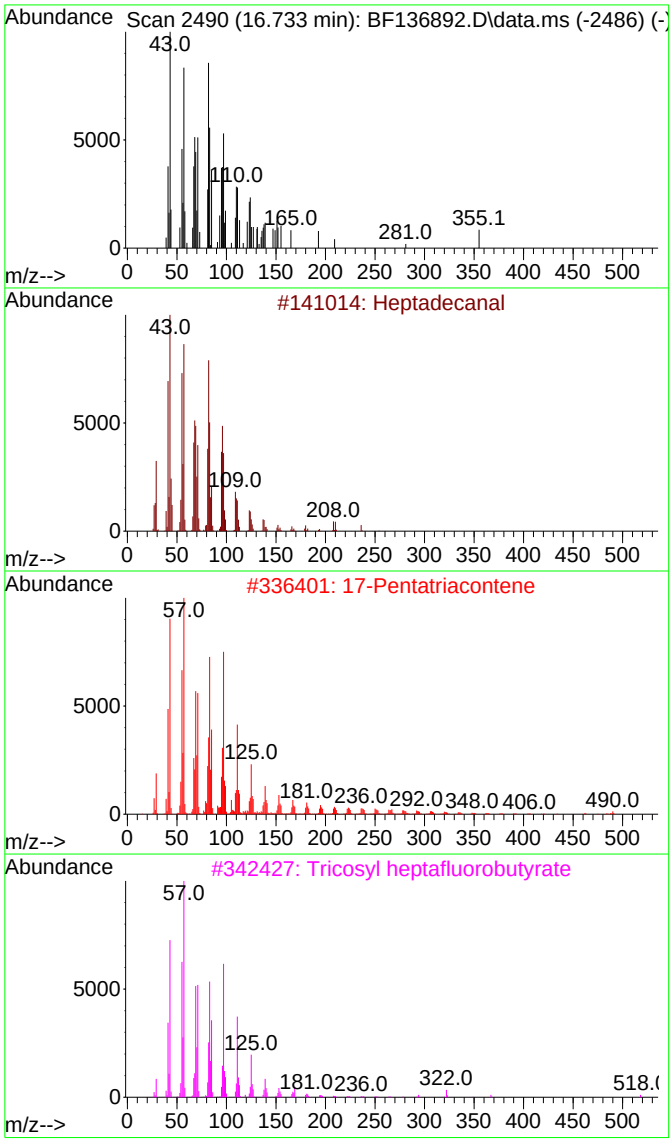
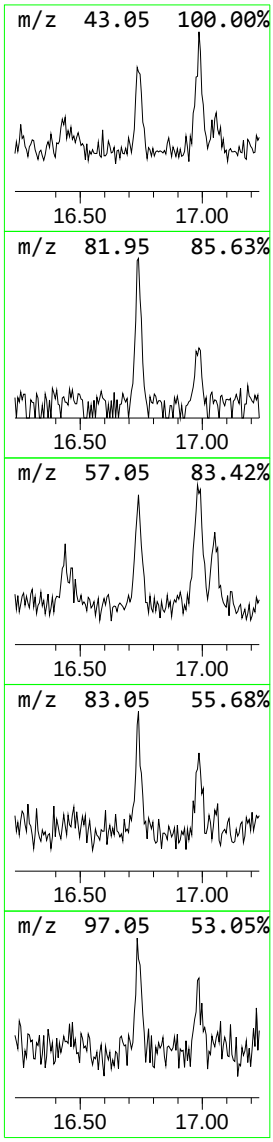
Peak Number 9 Heptadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	2.26 ng	47250	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanal	254	C17H34O	1000376-70-0	58
2	17-Pentatriacontene	491	C35H70	006971-40-0	49
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	43
4	Isobutyl tetratriacontyl ether	551	C38H78O	1000406-33-7	43
5	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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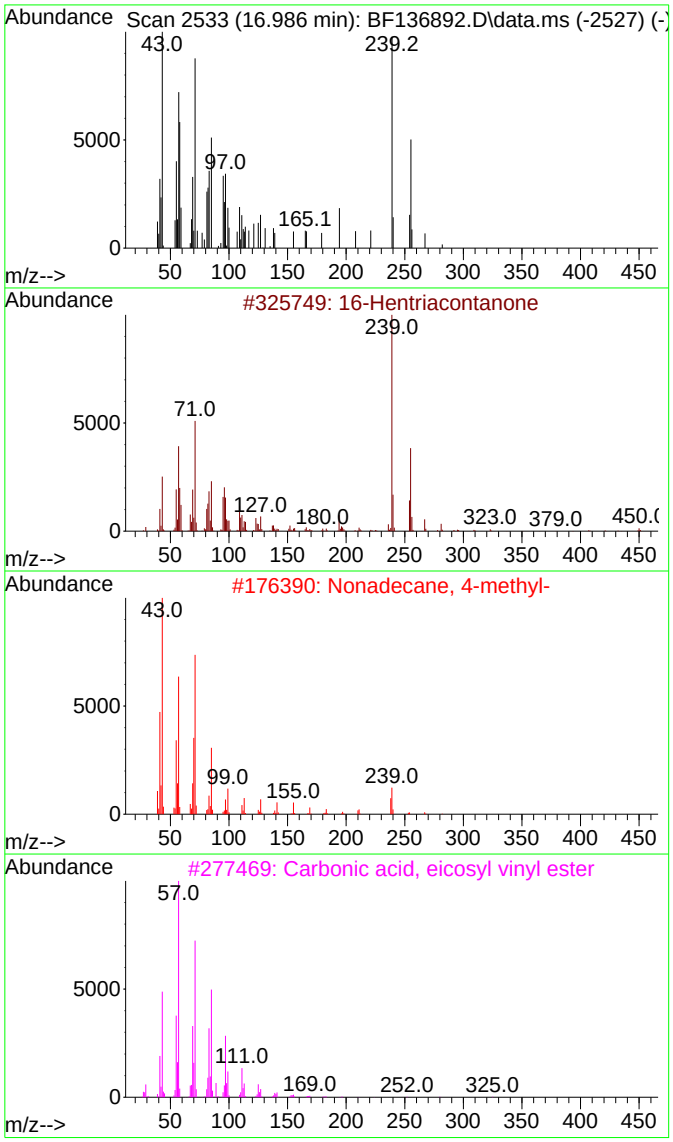
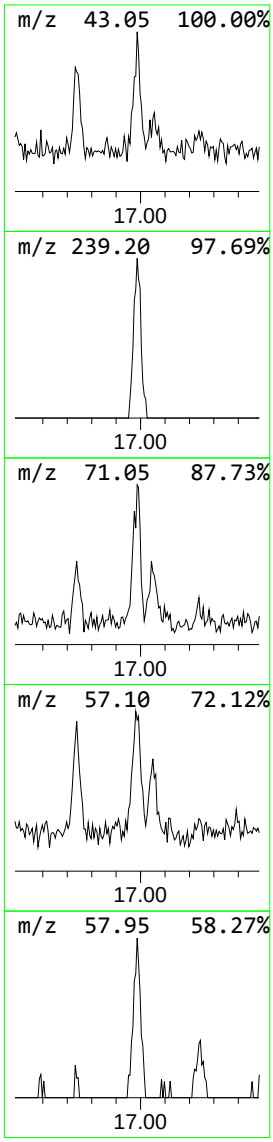
Peak Number 10 16-Hentriacontanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.986	2.61 ng	54503	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Hentriacontanone	450	C31H62O	000502-73-8	50
2	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	49
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35
4	Isobutyl hexadecyl ether	298	C20H42O	1000406-32-8	35
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136892.D
Acq On : 03 Jan 2024 02:09
Operator : CG\JU
Sample : 05900-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
n-Hexadecanoic ...	11.839	8.9	ng	253749	4	11.304	571445	20.0
cis-Vaccenic acid	12.551	3.3	ng	95497	4	11.304	571445	20.0
Octadecanoic acid	12.627	2.8	ng	79088	4	11.304	571445	20.0
Acetic acid n-o...	13.857	4.5	ng	83583	5	13.957	375476	20.0
5-Ethyl-5-methy...	14.433	2.3	ng	42864	5	13.957	375476	20.0
Squalene	14.815	4.7	ng	98805	6	15.439	417458	20.0
Heptadecane	15.080	2.2	ng	45582	6	15.439	417458	20.0
Pentadecanal-	15.674	2.7	ng	56705	6	15.439	417458	20.0
Heptadecanal	16.733	2.3	ng	47250	6	15.439	417458	20.0
16-Hentriaconta...	16.986	2.6	ng	54503	6	15.439	417458	20.0