LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134596.D
Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-P2A

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	494	497	503	rVB	59589	66468	3.32%	0.348%
2	5.416	561	566	569	rBV	2259704	1991376	99.57%	10.430%
3	6.422	732	737	740	rBV	2096186	2000027	100.00%	10.475%
4	6.792	797	800	804	rVB	1294001	1049757	52.49%	5.498%
5	7.351	890	895	898	rBV	1525944	1201859	60.09%	6.295%
6	8.069	1013	1017	1021	rBV	1597703	1342842	67.14%	7.033%
7	9.145	1196	1200	1204	rBV	2264254	1889418	94.47%	9.896%
8	9.269	1217	1221	1225	rBV	45053	41003	2.05%	0.215%
9	9.828	1312	1316	1319	rBV	1440724	1246337	62.32%	6.527%
10	9.951	1334	1337	1341	rBV	27456	26132	1.31%	0.137%
11	10.204	1375	1380	1383	rBV	41685	33393	1.67%	0.175%
12	10.610	1445	1449	1453	rBV	1197095	959906	47.99%	5.027%
13	10.651	1453	1456	1459	rVB4	22714	27757	1.39%	0.145%
14	10.751	1467	1473	1478	rBV2	81513	97777	4.89%	0.512%
15	11.316	1562	1569	1572	rBV	1270221	1196807	59.84%	6.268%
16	11.851	1656	1660	1664	rBV	197297	183216	9.16%	0.960%
17	12.033	1687	1691	1696	rBV3	24573	29061	1.45%	0.152%
18	12.527	1769	1775	1778	rBV	54525	61529	3.08%	0.322%
19	12.639	1791	1794	1803	rBV5	47429	62063	3.10%	0.325%
20	12.751	1808	1813	1817	rBV	61580	70308	3.52%	0.368%
21	12.904	1835	1839	1843	rBV	1788173	1579501	78.97%	8.272%
22	13.151	1879	1881	1884	rVB	37823	31704	1.59%	0.166%
23	13.192	1884	1888	1891	rBV3	17167	22714	1.14%	0.119%
24	13.280	1898	1903	1906	rBV4	19034	23654	1.18%	0.124%
25	13.498	1937	1940	1942	rVB	33221	29832	1.49%	0.156%
26	13.821	1991	1995	2003	rBV2	221612	279738	13.99%	1.465%
27	13.957	2014	2018	2021	rBV	1072235	910821	45.54%	4.770%
28	14.145	2047	2050	2058	rVB	54624	54990	2.75%	0.288%
29	14.457	2098	2103	2107	rBV	157245	203318	10.17%	1.065%
30	14.762	2152	2155	2161	rVB2	45939	56207	2.81%	0.294%
31	14.904	2177	2179	2183	rVB3	57426	54170	2.71%	0.284%
32	15.104	2209	2213	2215	rBV	101816	117188	5.86%	0.614%
33	15.127	2215	2217	2222	rVB	114266	133853	6.69%	0.701%
34	15.421	2262	2267	2271	rVB	532775	628784	31.44%	3.293%
35	15.698	2310	2314	2318	rBV2	70301	96773	4.84%	0.507%
36	15.939	2351	2355	2359	rBV	70515	105829	5.29%	0.554%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
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Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.992	2359	2364	2373	rVB3	125100	233757	11.69%	1.224%
38	17.533	2619	2626	2638	rBV2	195572	499278	24.96%	2.615%
39	18.109	2717	2724	2733	rVB2	71480	178804	8.94%	0.936%
40	18.362	2760	2767	2771	rBV9	25044	65532	3.28%	0.343%
41	18.580	2798	2804	2817	rVB4	76316	210184	10.51%	1.101%

Sum of corrected areas: 19093667

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
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Instrument :
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ClientSampleId :
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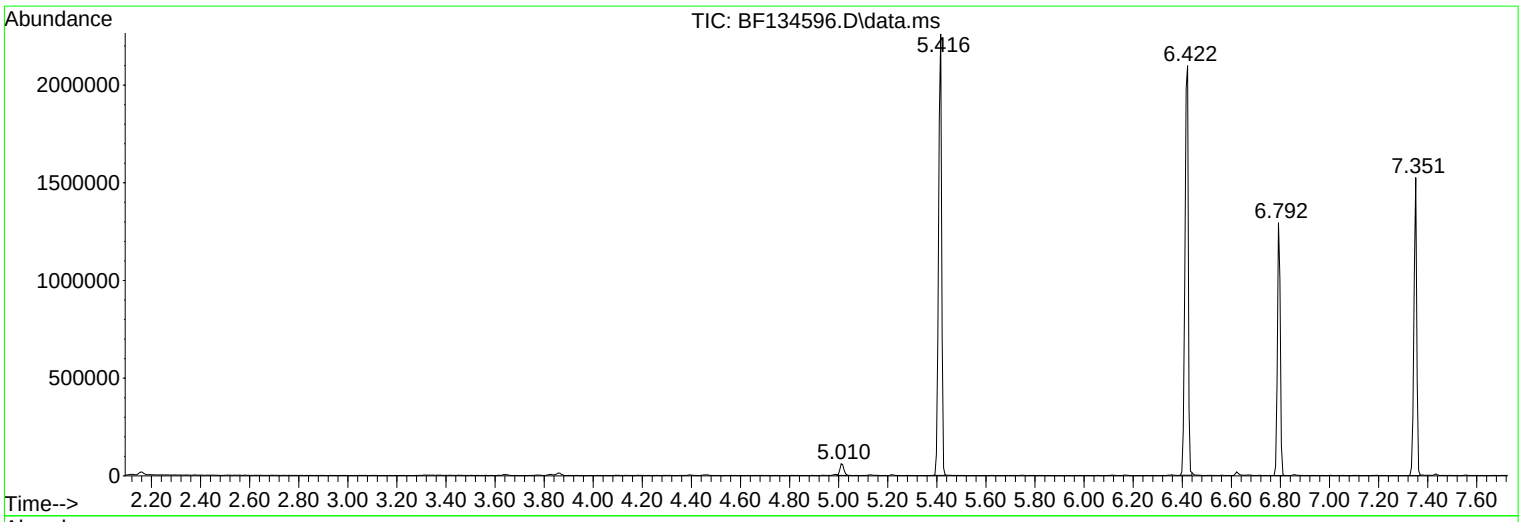
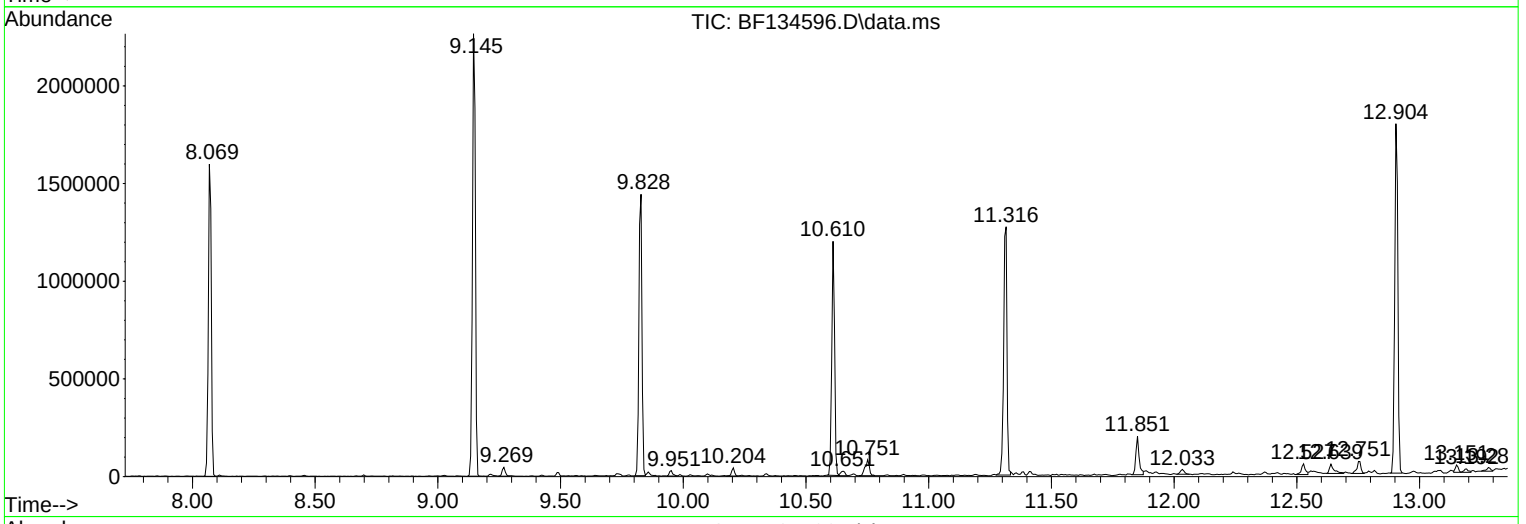
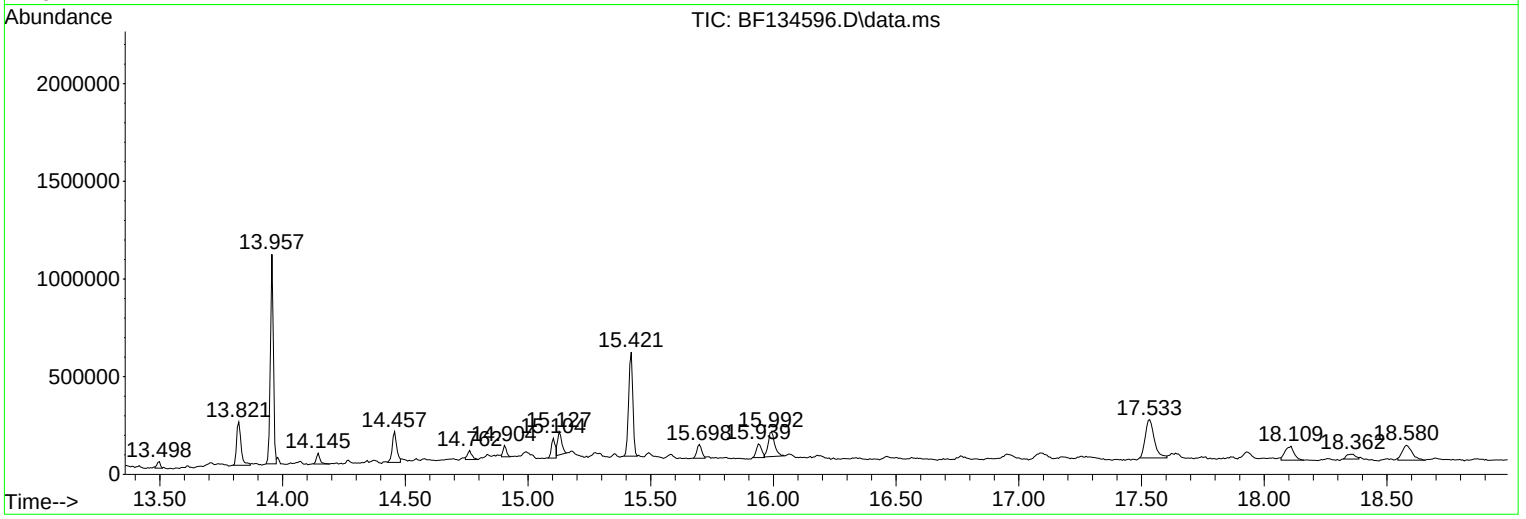
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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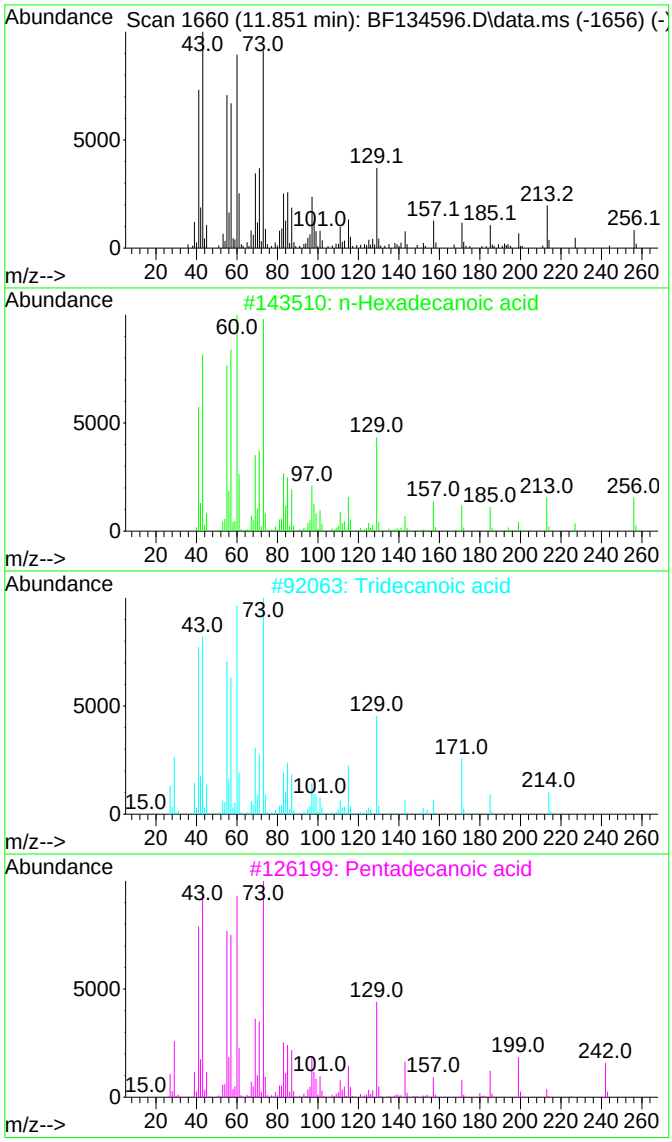
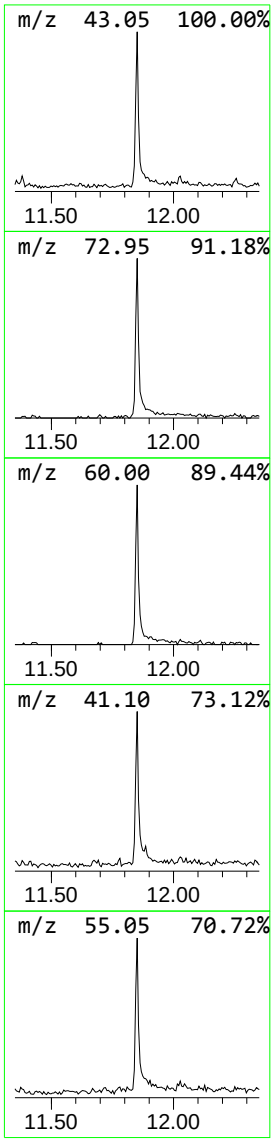
Peak Number 1 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	3.06 ng	183216	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Sample : 03834-01
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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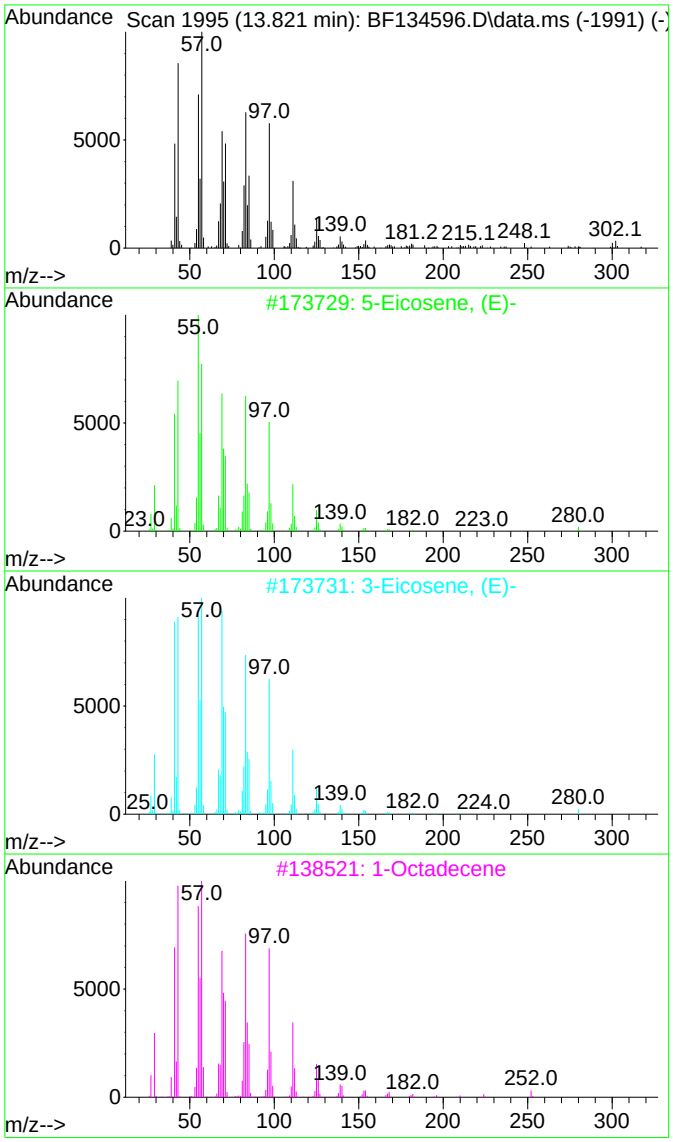
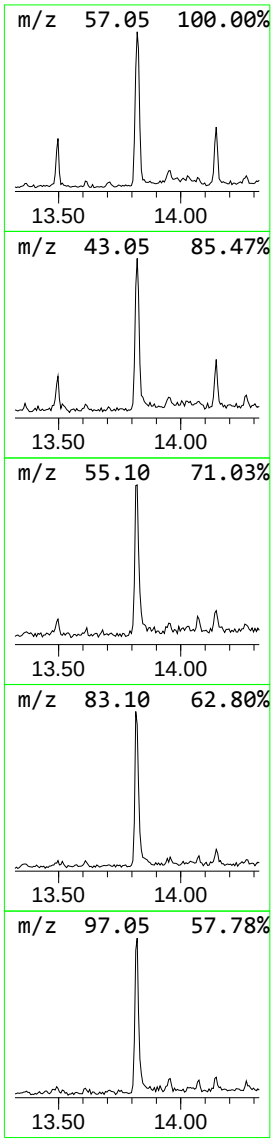
Peak Number 2 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	6.14 ng	279738	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	1-Octadecene	252	C18H36	000112-88-9	95
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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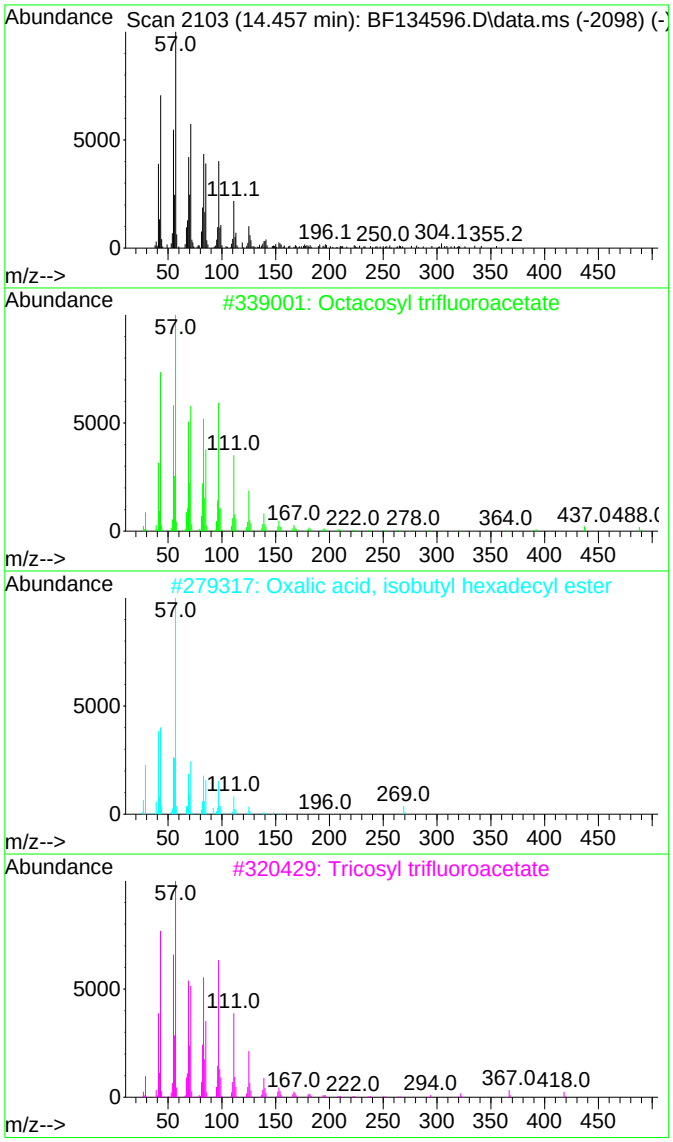
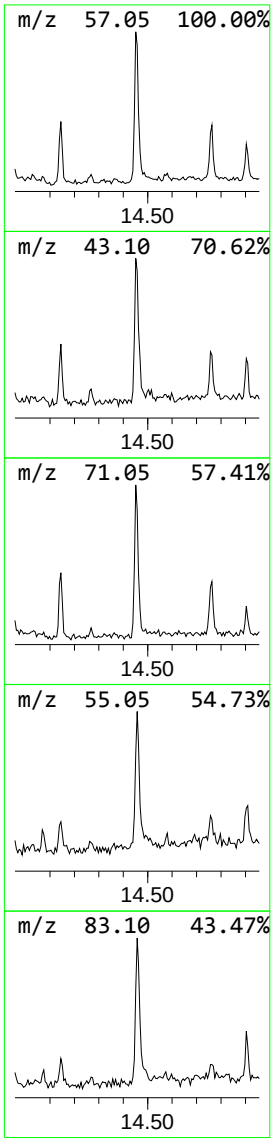
Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	4.46 ng	203318	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4	Cyclopentadecane	210	C15H30	000295-48-7	90
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134596.D
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Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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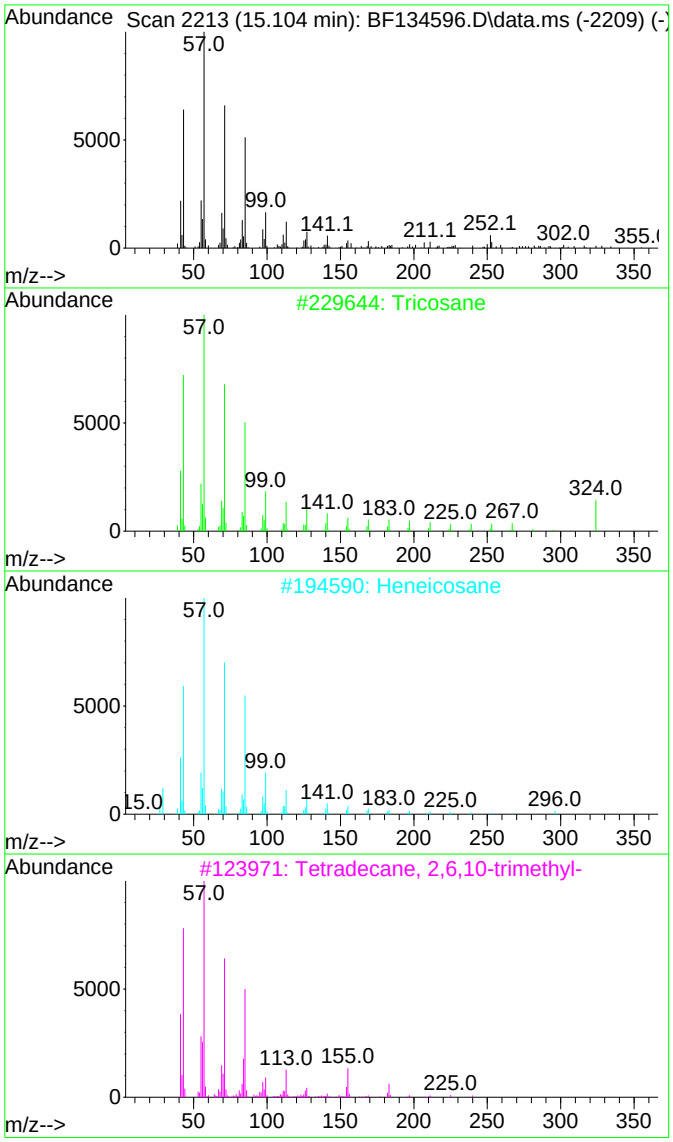
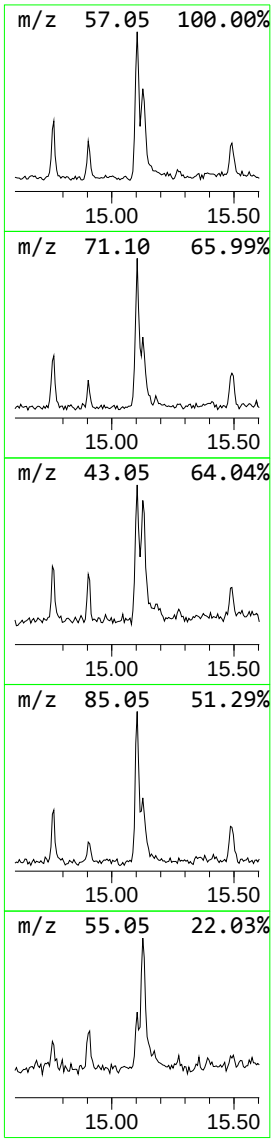
Peak Number 4 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	3.73 ng	117188	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Nonadecane	268	C19H40	000629-92-5	83





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Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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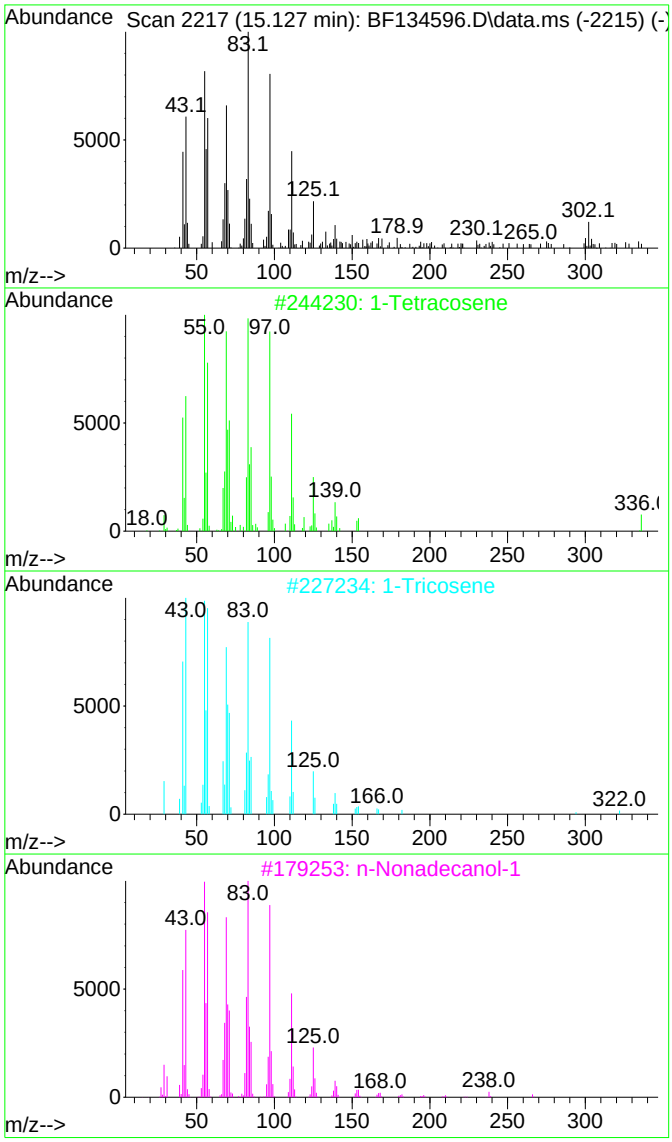
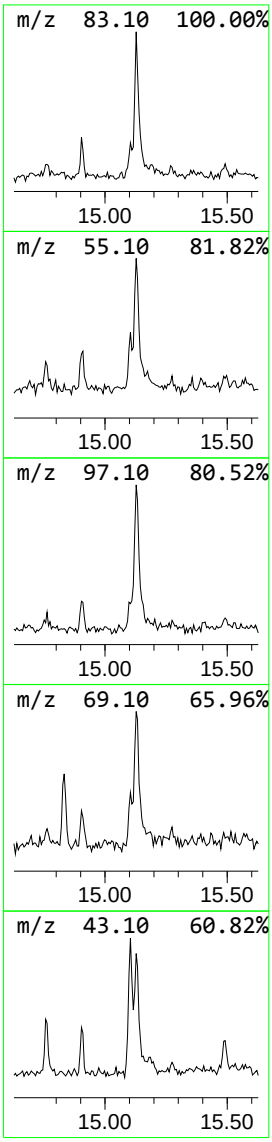
Peak Number 5 1-Tetracosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	4.26 ng	133853	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	91
2	1-Tricosene	322	C23H46	018835-32-0	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	80
4	1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	80
5	Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	62





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Operator : CG\JU
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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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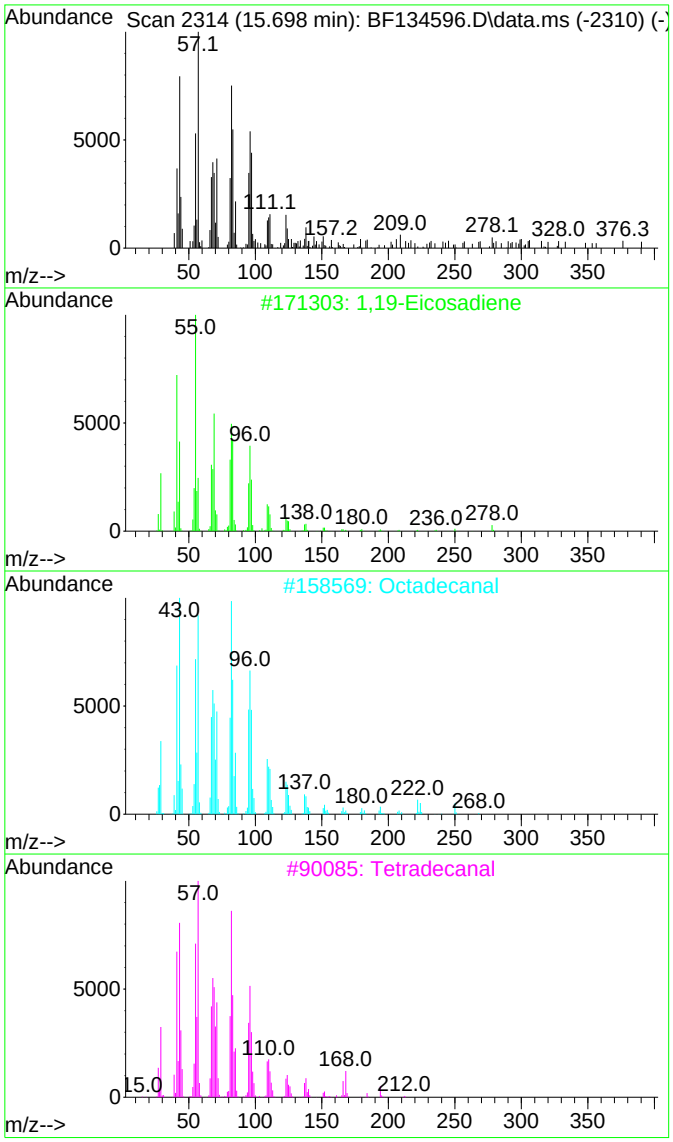
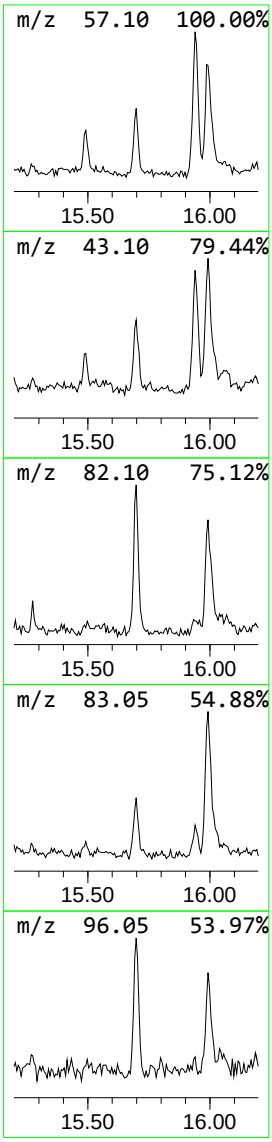
Peak Number 6 1,19-Eicosadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	3.08 ng	96773	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	92
2	Octadecanal	268	C18H36O	000638-66-4	90
3	Tetradecanal	212	C14H28O	000124-25-4	83
4	Hexadecanal	240	C16H32O	000629-80-1	80
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74





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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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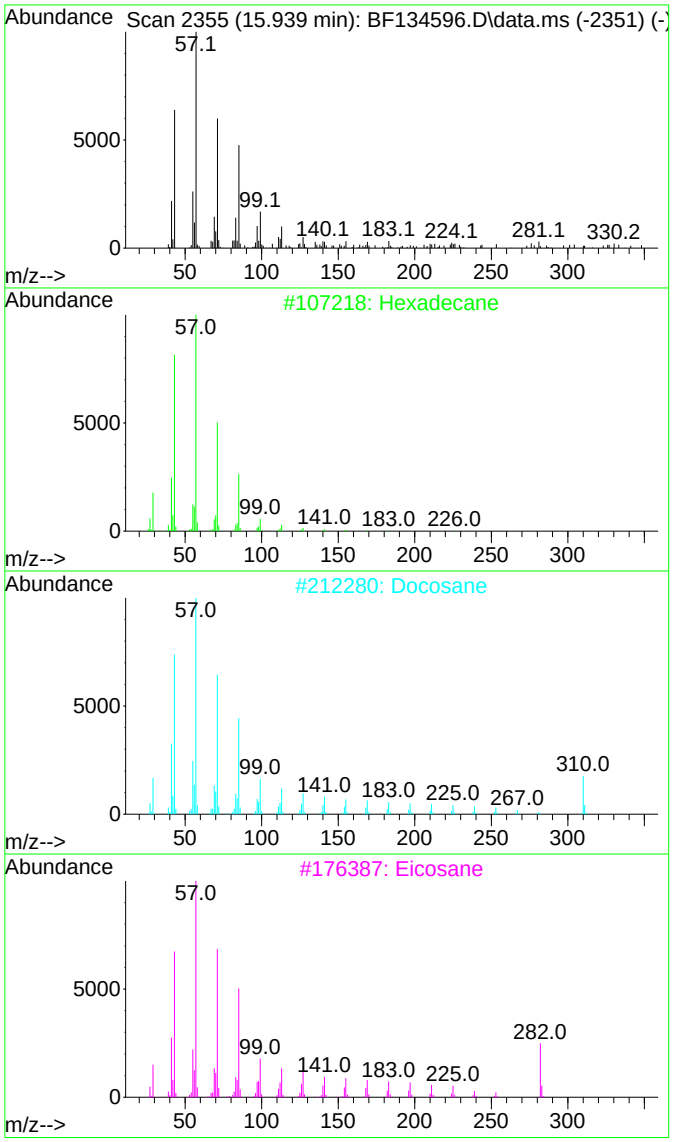
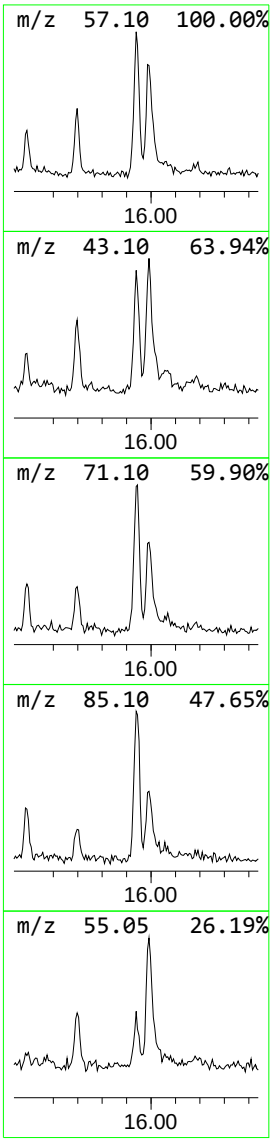
Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	3.37 ng	105829	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Docosane	310	C22H46	000629-97-0	80
3	Eicosane	282	C20H42	000112-95-8	80
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	80





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ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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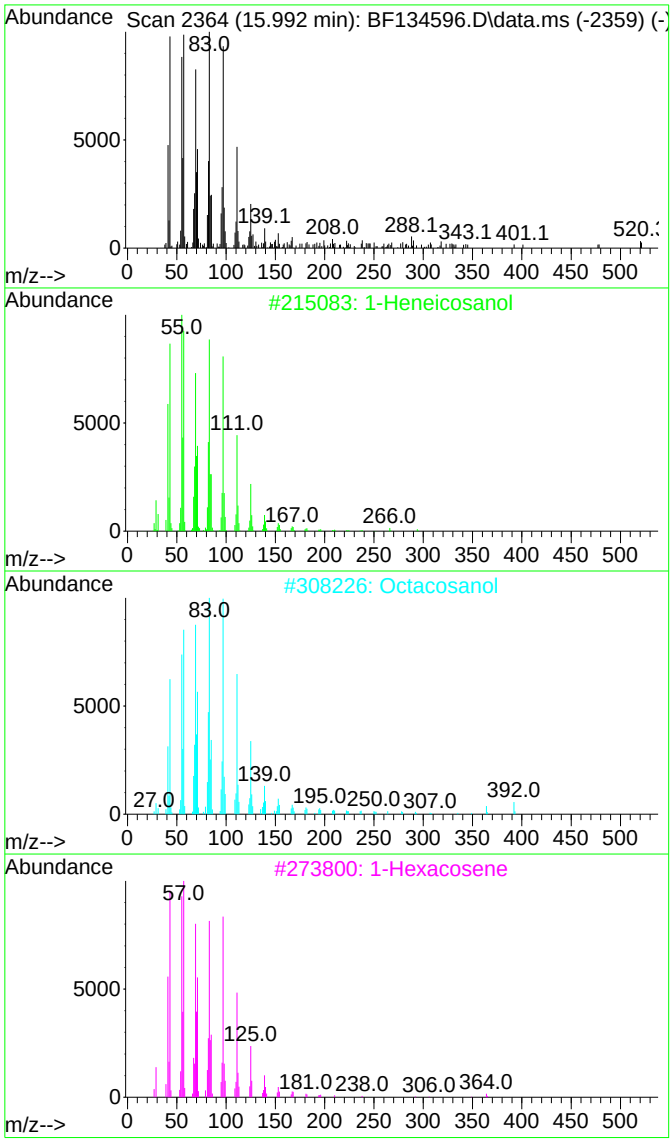
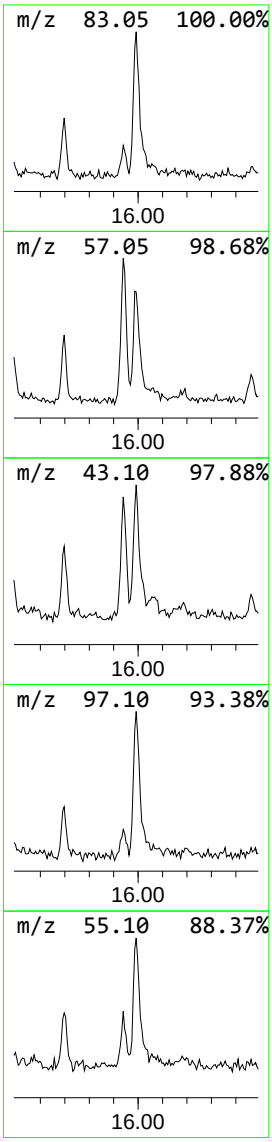
Peak Number 8 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	7.44 ng	233757	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Octacosanol	410	C28H58O	000557-61-9	91
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83





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Misc :
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Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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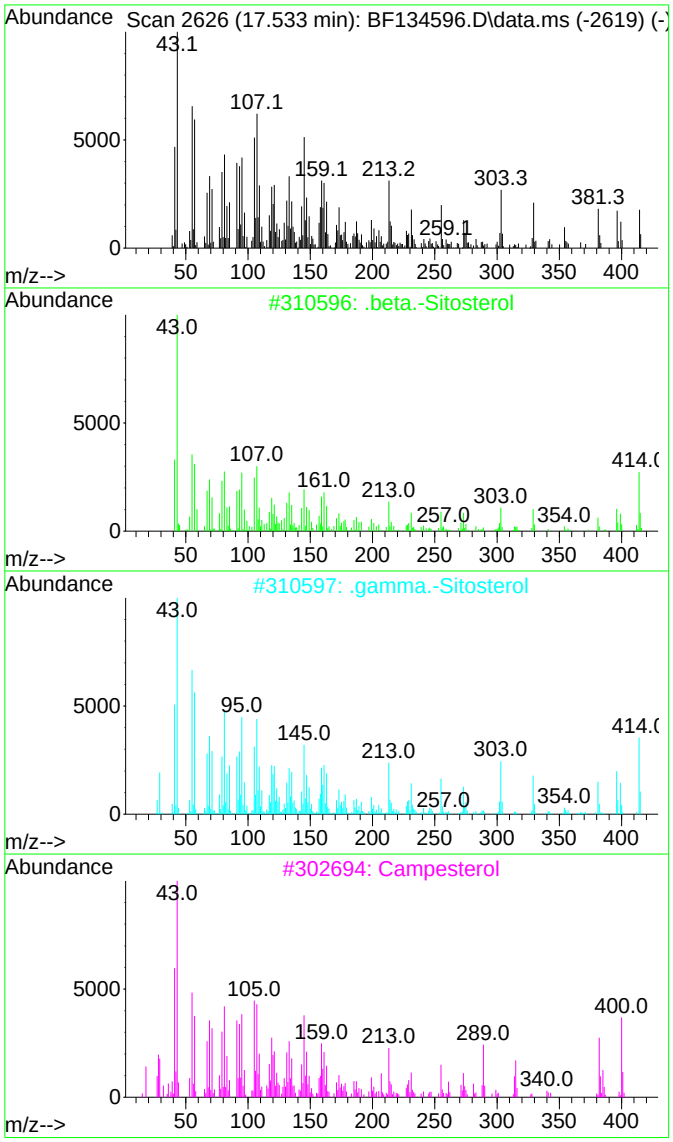
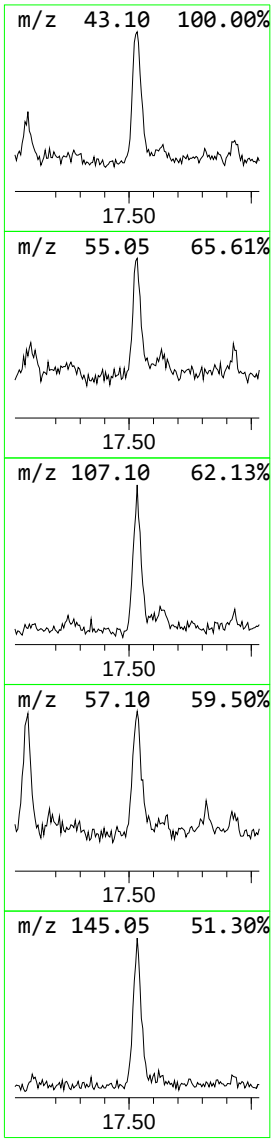
Peak Number 9 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.533	15.88 ng	499278	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	97
3	Campesterol	400	C28H48O	000474-62-4	49
4	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	43
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	35





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Data File : BF134596.D
Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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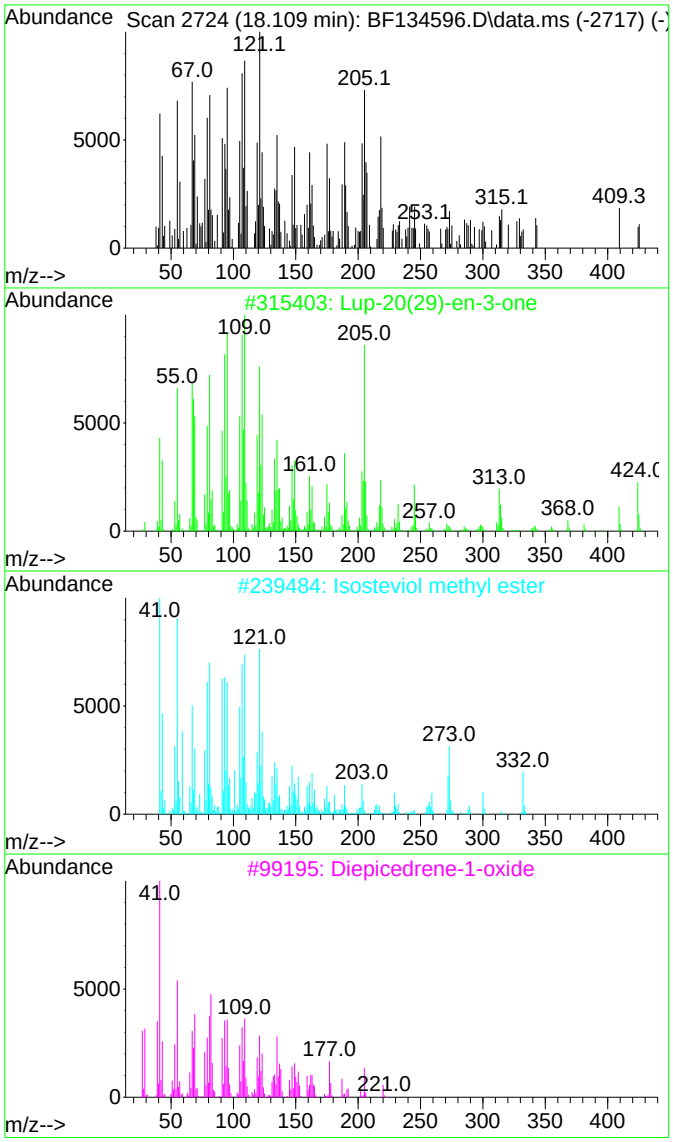
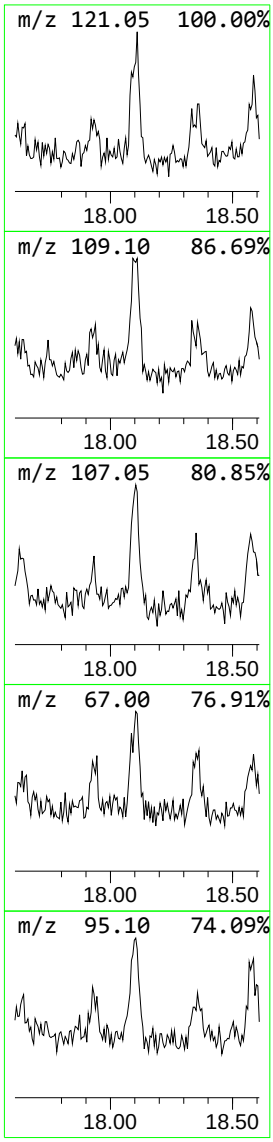
Peak Number 10 Lup-20(29)-en-3-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	5.69 ng	178804	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	97
2	Isosteviol methyl ester	332	C21H32O3	1000256-08-8	62
3	Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	60
4	.beta.-Amyrone	424	C30H48O	000638-97-1	50
5	13,15-Octacosadiyne	386	C28H50	024643-46-7	46





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Data File : BF134596.D
Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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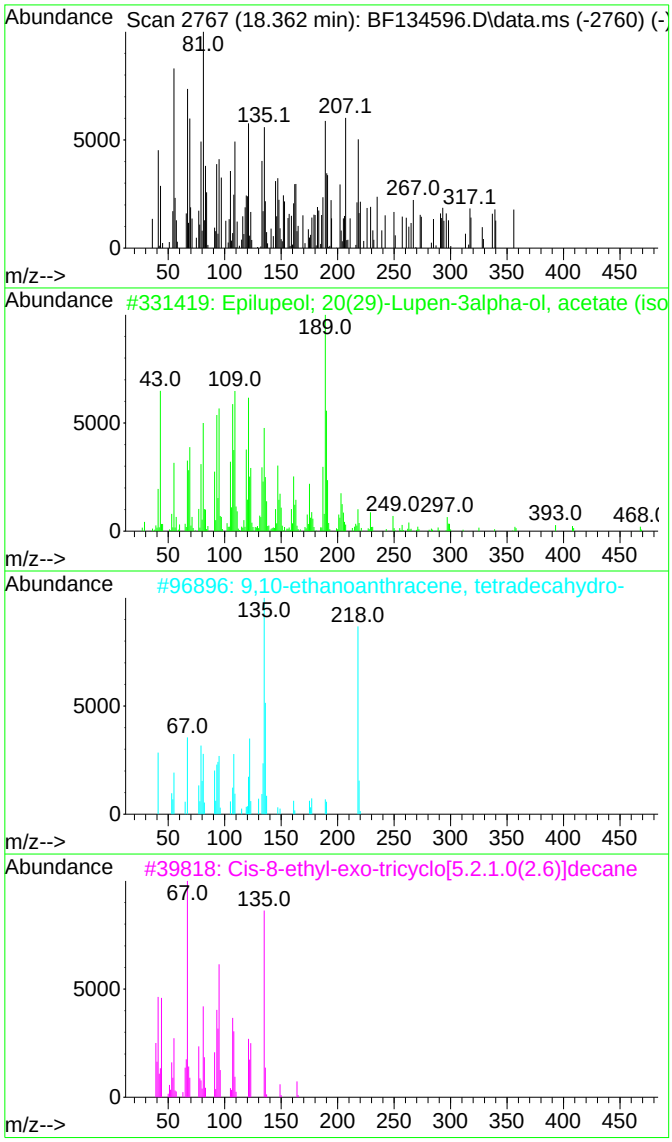
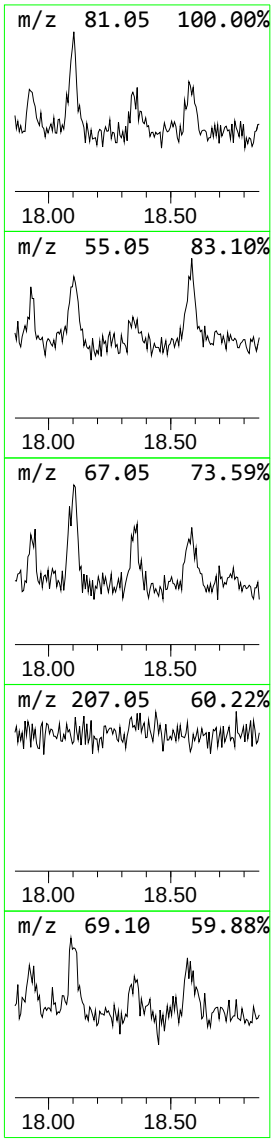
Peak Number 11 unknown18.362 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	2.08 ng	65532	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	38
2	9,10-ethanoanthracene, tetradeca...	218	C16H26	1000396-23-0	30
3	Cis-8-ethyl-exo-tricyclo[5.2.1.0...	164	C12H20	1000215-29-4	25
4	Bi-1-cycloocten-1-yl	218	C16H26	061468-42-6	25
5	Methyl 2-(4-fluorophenyl)cyclopr...	194	C11H11FO2	1010445-26-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134596.D
Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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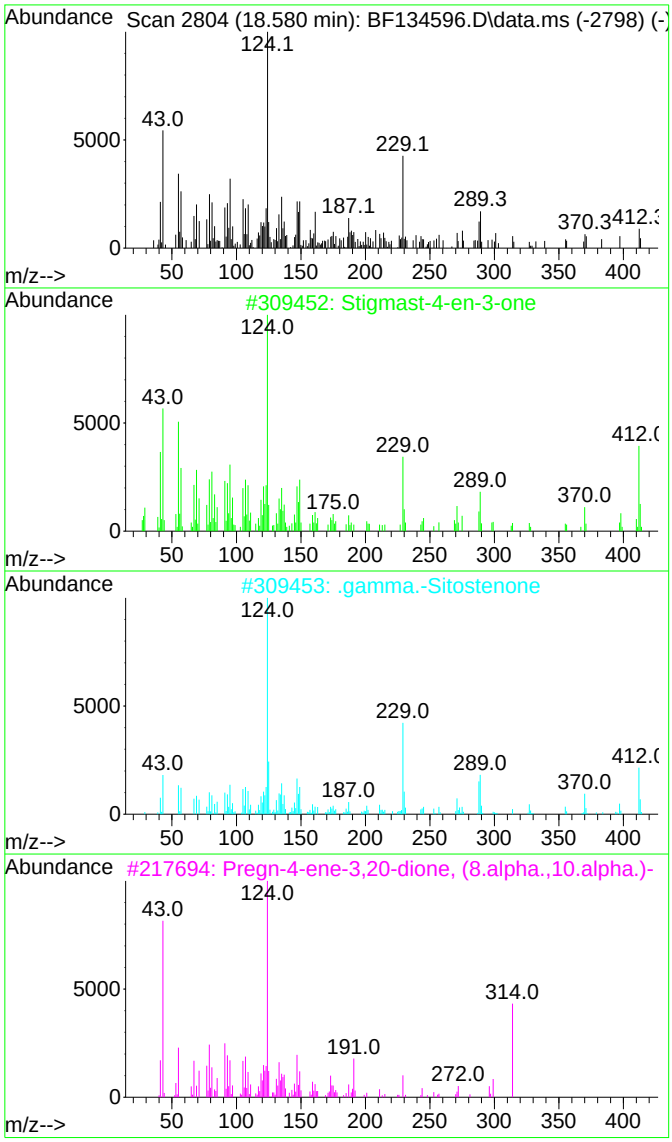
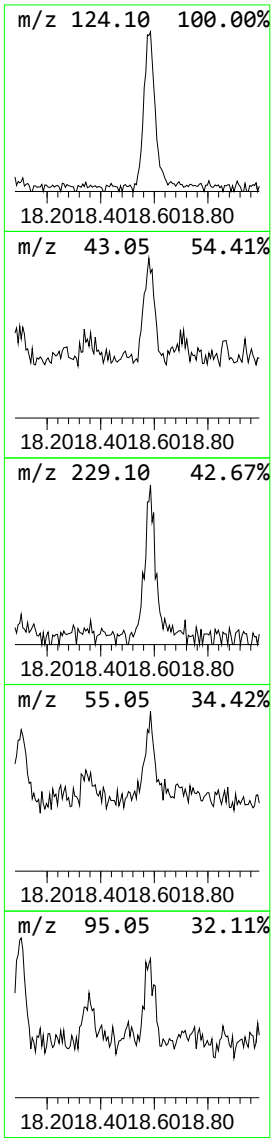
Peak Number 12 Stigmast-4-en-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.580	6.69 ng	210184	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	96
2	.gamma.-Sitostenone	412	C29H48O	084924-96-9	81
3	Pregn-4-ene-3,20-dione, (8.alpha...	314	C21H30O2	003795-19-5	70
4	Testosterone	288	C19H28O2	000058-22-0	60
5	Cyclobuta[1,2:3,4]dicyclooctene-...	248	C16H24O2	069926-83-6	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134596.D
Acq On : 02 Aug 2023 23:52
Operator : CG\JU
Sample : 03834-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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 ...	11.851	3.1	ng	183216	4	11.316	1196810	20.0
5-Eicosene, (E)-	13.821	6.1	ng	279738	5	13.957	910821	20.0
Octacosyl trifl...	14.457	4.5	ng	203318	5	13.957	910821	20.0
Tricosane	15.104	3.7	ng	117188	6	15.421	628784	20.0
1-Tetracosene	15.127	4.3	ng	133853	6	15.421	628784	20.0
1,19-Eicosadiene	15.698	3.1	ng	96773	6	15.421	628784	20.0
Hexadecane	15.939	3.4	ng	105829	6	15.421	628784	20.0
1-Heneicosanol	15.992	7.4	ng	233757	6	15.421	628784	20.0
.beta.-Sitosterol	17.533	15.9	ng	499278	6	15.421	628784	20.0
Lup-20(29)-en-3...	18.109	5.7	ng	178804	6	15.421	628784	20.0
unknown18.362	18.362	2.1	ng	65532	6	15.421	628784	20.0
Stigmast-4-en-3...	18.580	6.7	ng	210184	6	15.421	628784	20.0