LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
Data File : BF127813.D
Acq On : 15 Apr 2022 19:52
Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.569	553	558	561	rBV	2566978	2418053	3.58%	1.236%
2	6.569	722	728	731	rBV	2222335	2317384	3.43%	1.185%
3	6.946	788	792	796	rBV	986858	813167	1.21%	0.416%
4	7.510	883	888	891	rBV	1809308	1559698	2.31%	0.797%
5	8.234	1007	1011	1014	rBV	961781	905766	1.34%	0.463%
6	9.304	1189	1193	1196	rBV	3037621	2449724	3.63%	1.252%
7	9.986	1306	1309	1312	rBV	1009073	845936	1.25%	0.432%
8	10.775	1440	1443	1447	rVB	1492337	1306286	1.94%	0.668%
9	11.481	1559	1563	1565	rBV	1006844	838934	1.24%	0.429%
10	11.863	1625	1628	1631	rVB	1047447	800664	1.19%	0.409%
11	12.133	1646	1674	1697	rBV	11747687	67473093	100.00%	34.493%
12	12.557	1743	1746	1748	rBV	2722516	2579556	3.82%	1.319%
13	12.580	1748	1750	1756	rVB2	1854189	1584163	2.35%	0.810%
14	12.827	1767	1792	1793	rBV	11985856	64503165	95.60%	32.975%
15	12.892	1797	1803	1806	rVB	8657670	14173713	21.01%	7.246%
16	13.080	1831	1835	1838	rVB	2457521	2194696	3.25%	1.122%
17	13.545	1908	1914	1919	rBV	3184380	3991756	5.92%	2.041%
18	14.133	2011	2014	2017	rBV	749529	796598	1.18%	0.407%
19	14.186	2017	2023	2028	rVV	3599651	3943469	5.84%	2.016%
20	14.239	2028	2032	2038	rVV	1171609	1556623	2.31%	0.796%
21	14.292	2038	2041	2044	rVV	882092	979972	1.45%	0.501%
22	14.339	2044	2049	2051	rVV	5096445	5593365	8.29%	2.859%
23	14.369	2051	2054	2061	rVB2	2457822	3075609	4.56%	1.572%
24	14.433	2061	2065	2074	rVB	1958150	2059101	3.05%	1.053%
25	15.263	2202	2206	2210	rVB	1118962	1231116	1.82%	0.629%
26	15.651	2268	2272	2280	rVB	498897	718112	1.06%	0.367%
27	16.133	2349	2354	2359	rVB	722212	1091656	1.62%	0.558%
28	16.310	2379	2384	2393	rVB2	412017	691717	1.03%	0.354%
29	17.404	2563	2570	2584	rBV4	459332	1300995	1.93%	0.665%
30	17.851	2638	2646	2660	rVB2	642032	1820862	2.70%	0.931%

Sum of corrected areas: 195614949

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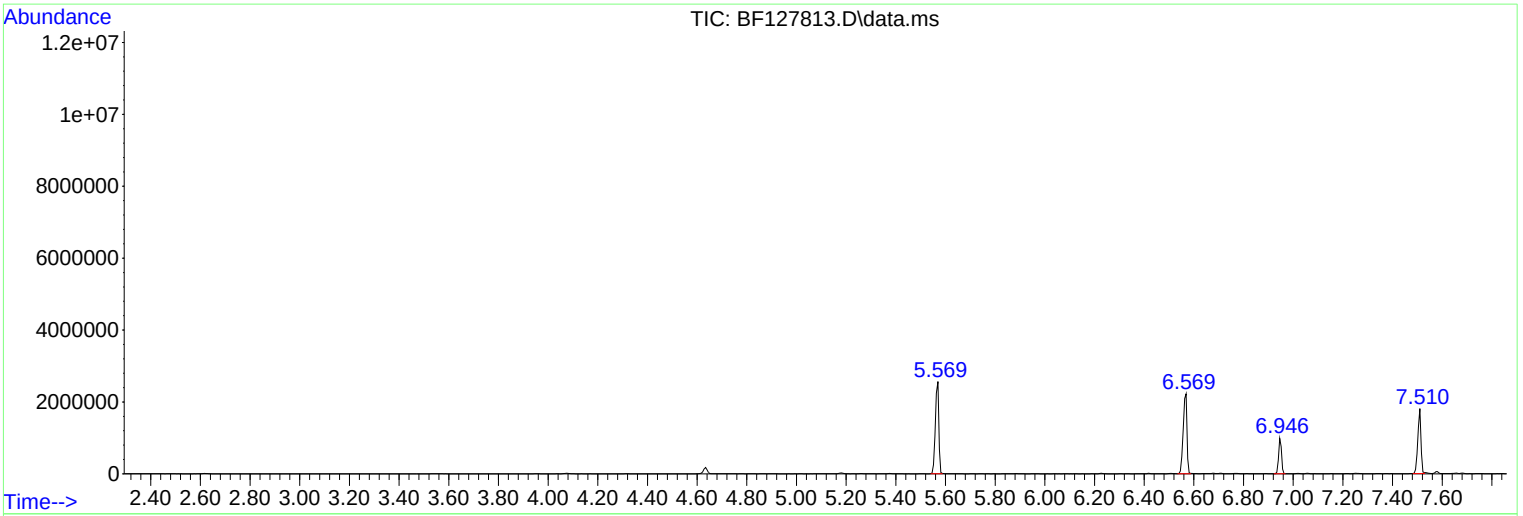
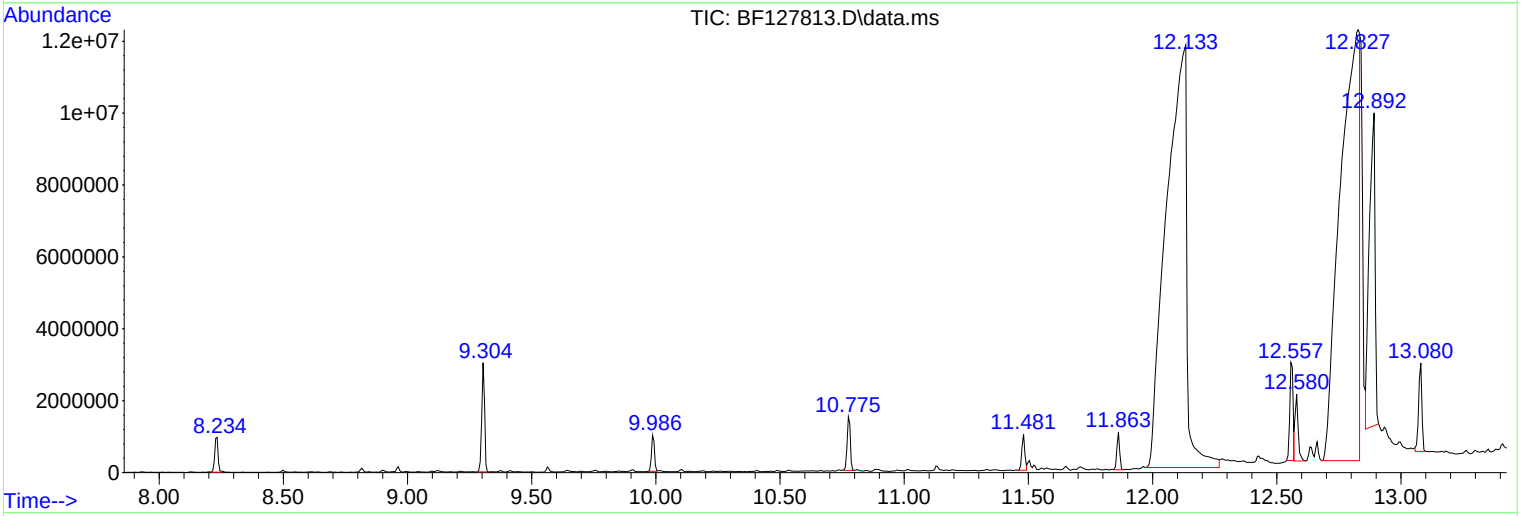
Misc :
ALS Vial : 18 Sample Multiplier: 1

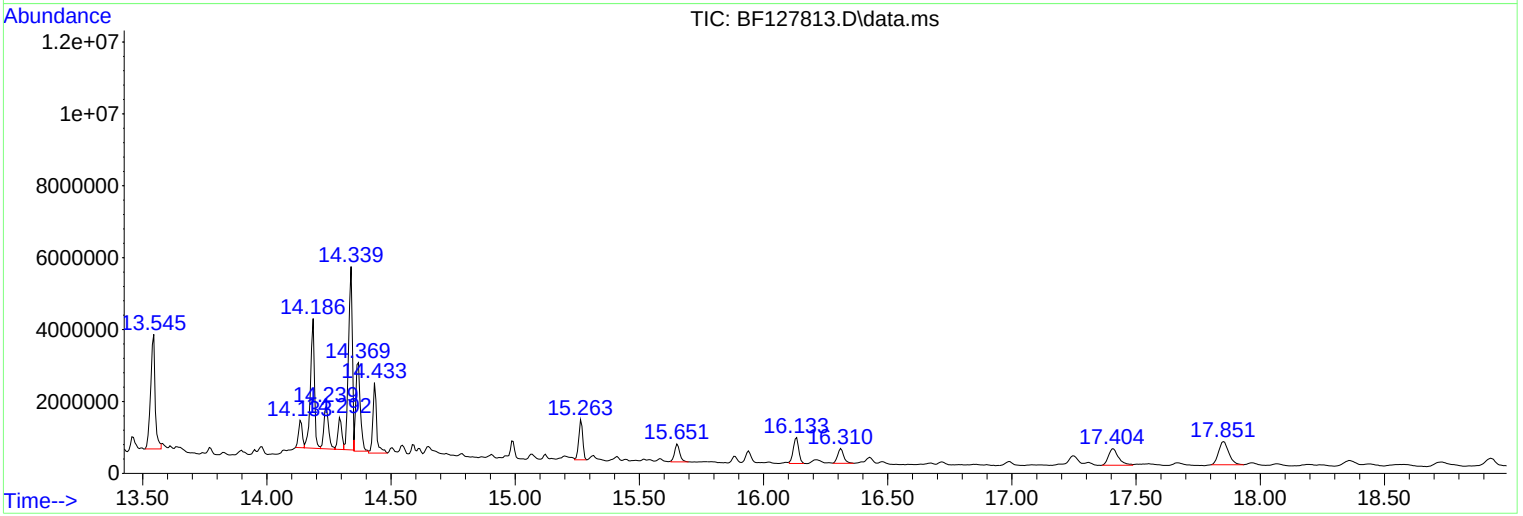
Instrument :
BNA_F
ClientSampleId :
BU-03-041422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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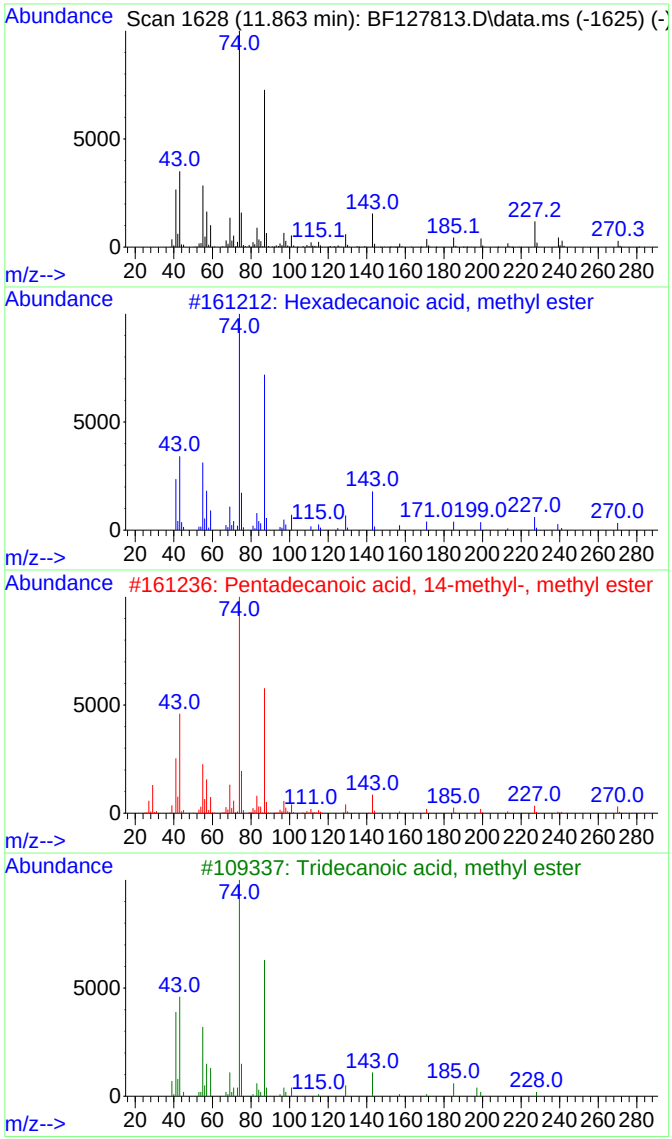
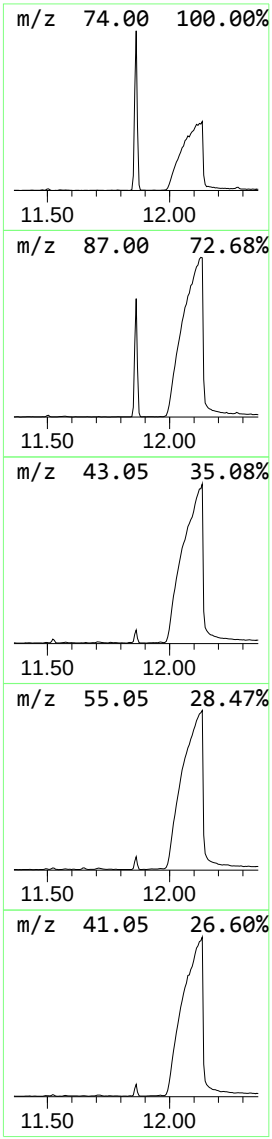
****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	19.09 ng	800664	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





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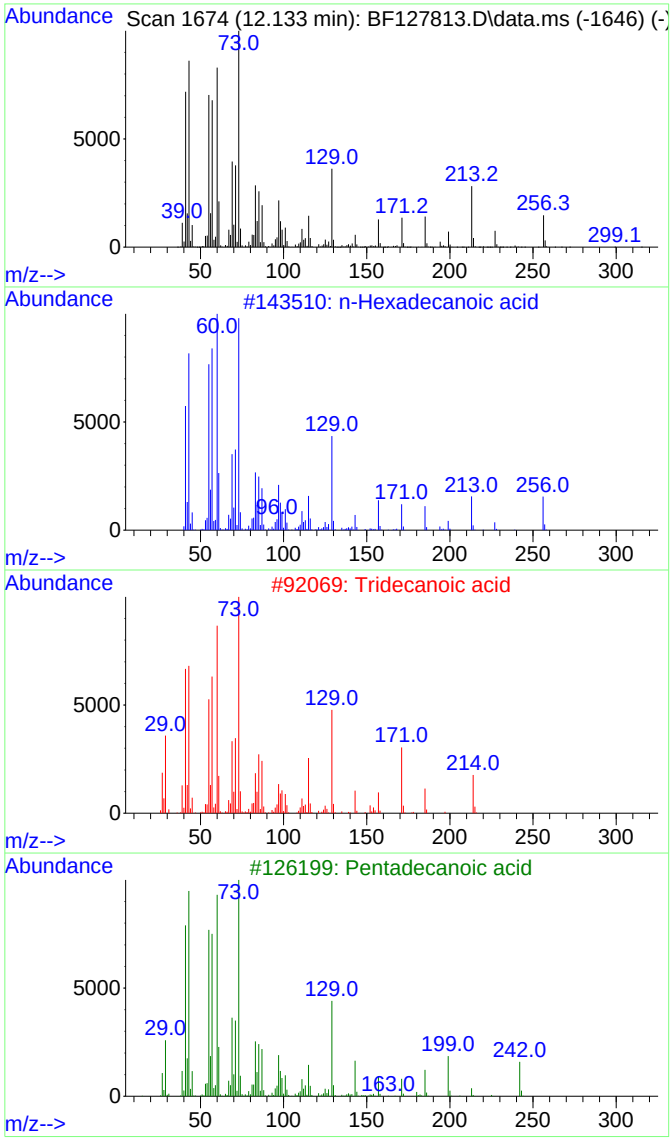
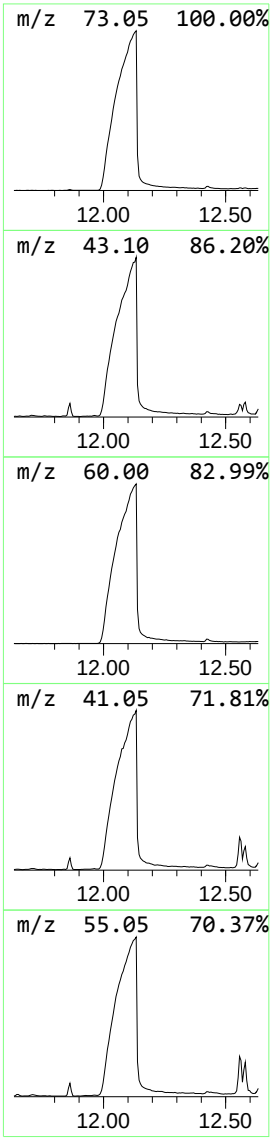
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.133	1608.54 ng	67473100	Phenanthrene-d10	11.480

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

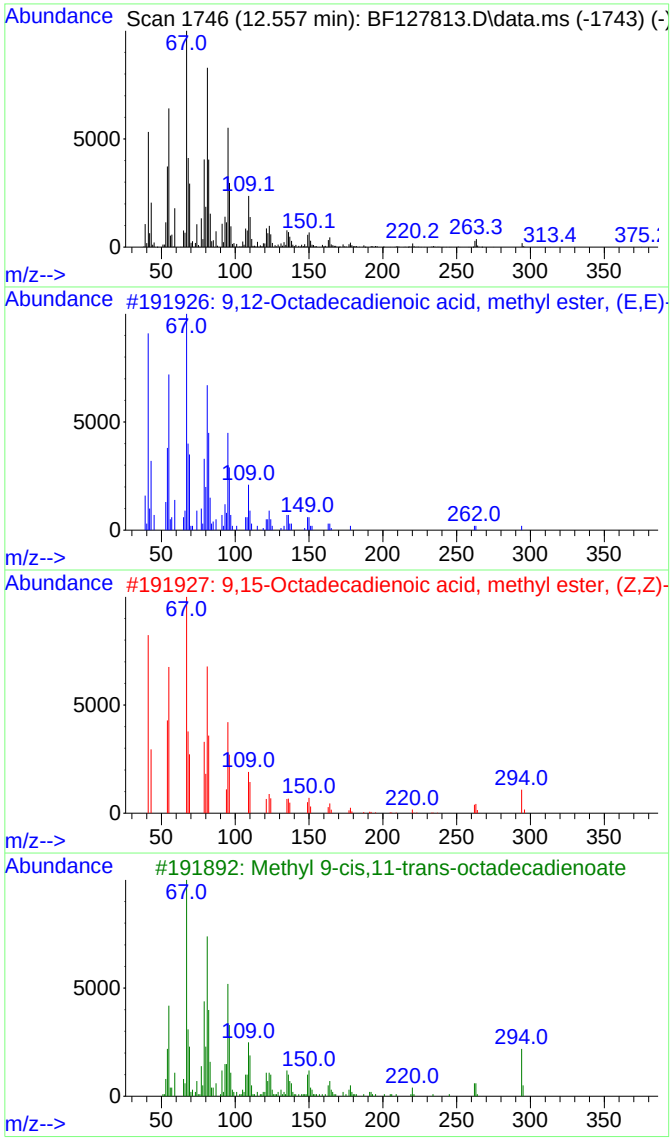
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

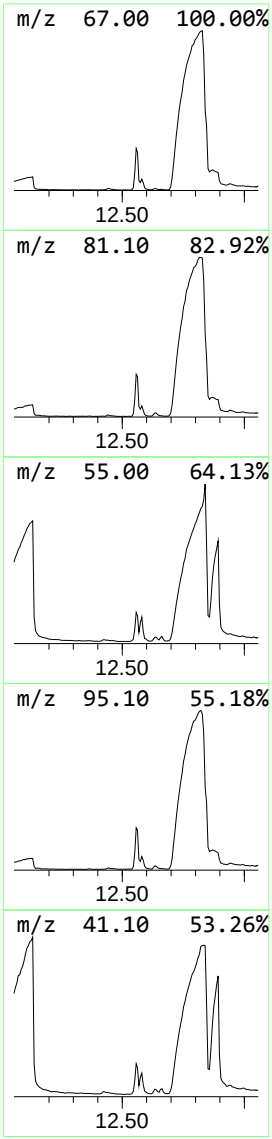
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	61.50 ng	2579560	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	95
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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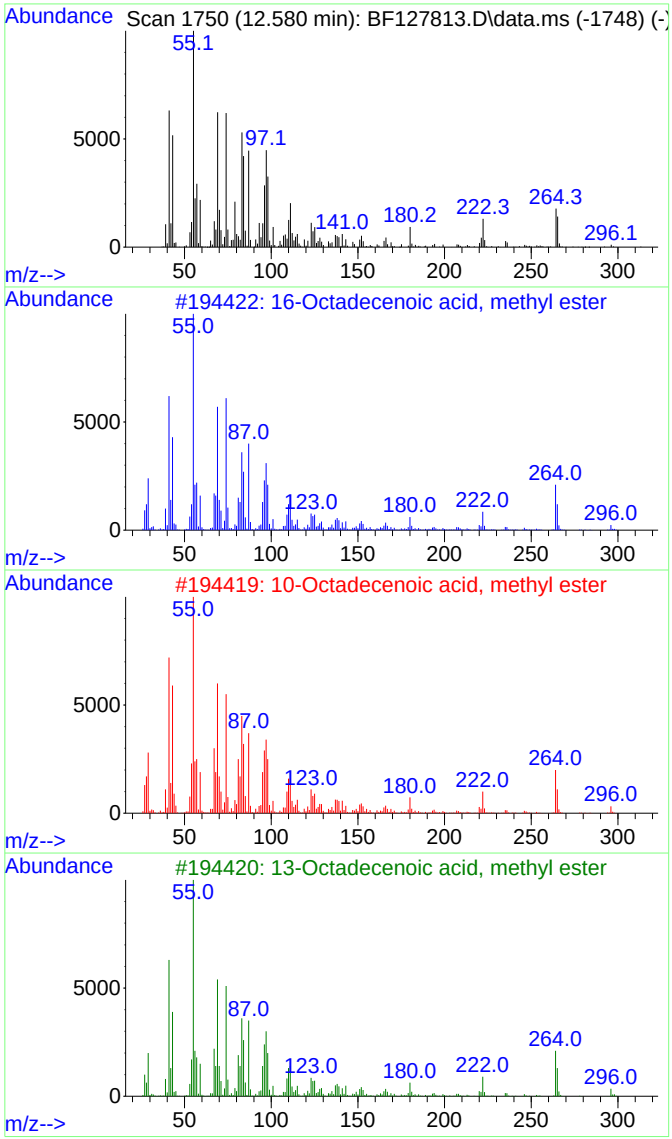
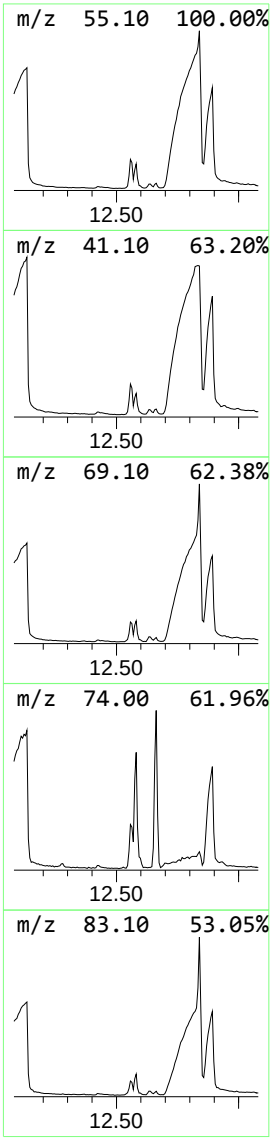
****
Peak Number 4 16-Octadecenoic acid, methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	37.77 ng	1584160	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	92
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	90
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	90





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TIC Library : C:\Database\NIST20.L
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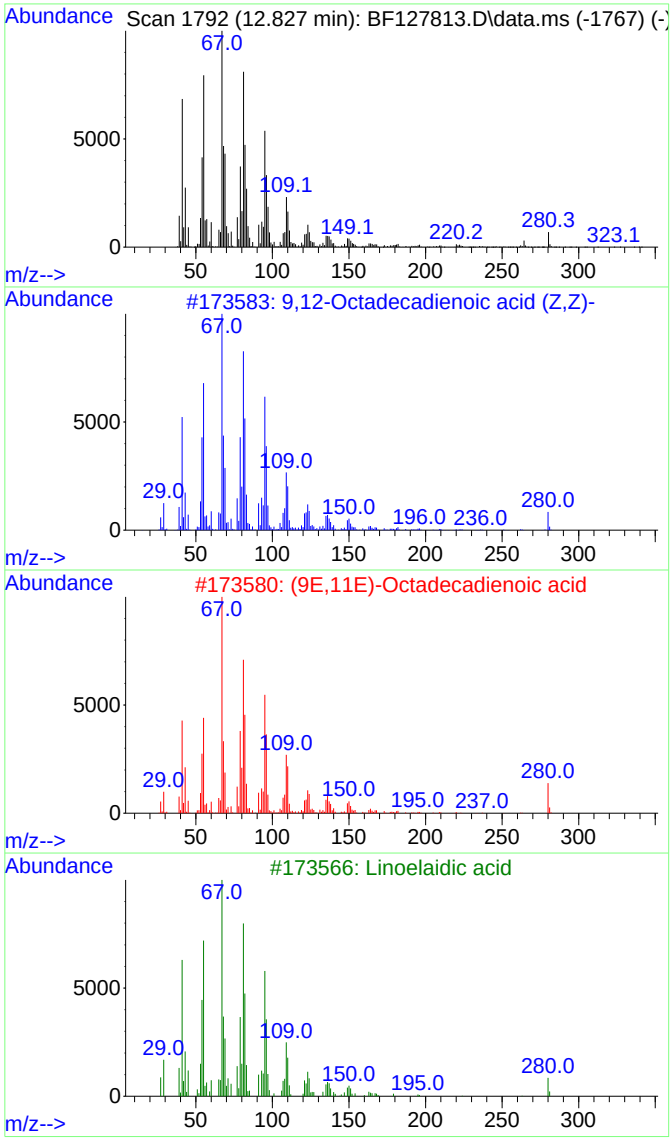
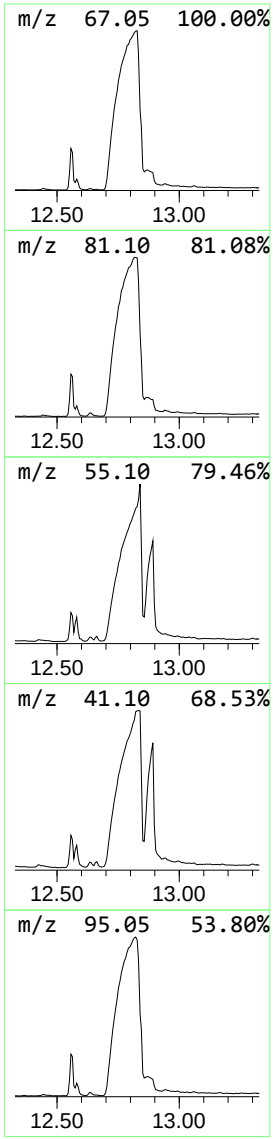
****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.828	1619.47 ng	64503200	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	99
3	Linoelaidic acid	280	C18H32O2	000506-21-8	99
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
5	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	92





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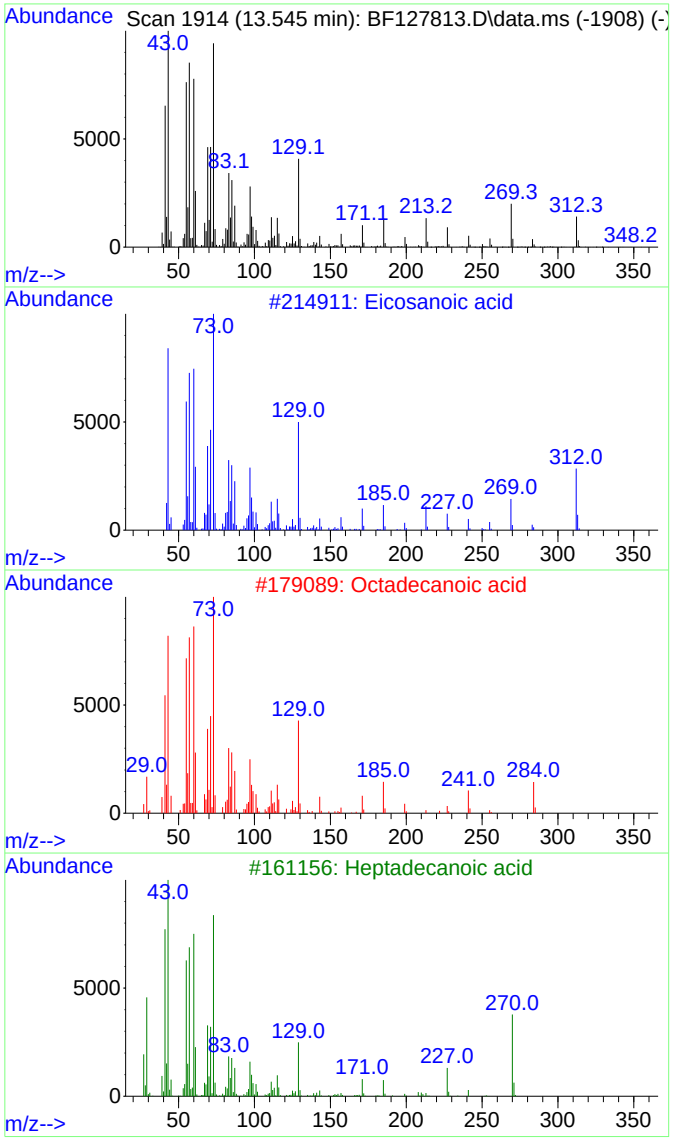
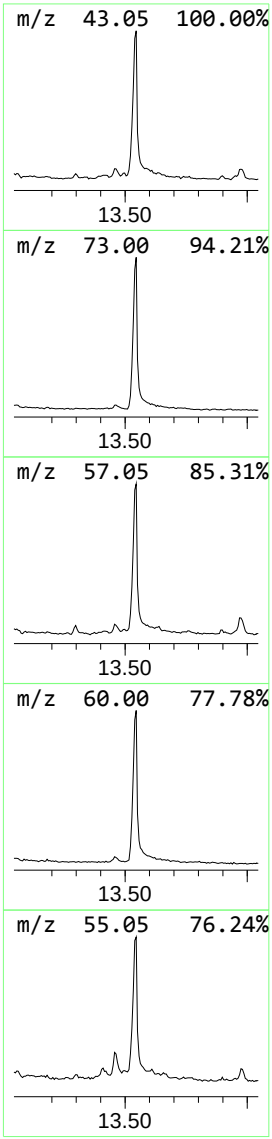
****

Peak Number 6 Eicosanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	100.22 ng	3991760	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid	312	C20H40O2	000506-30-9	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81





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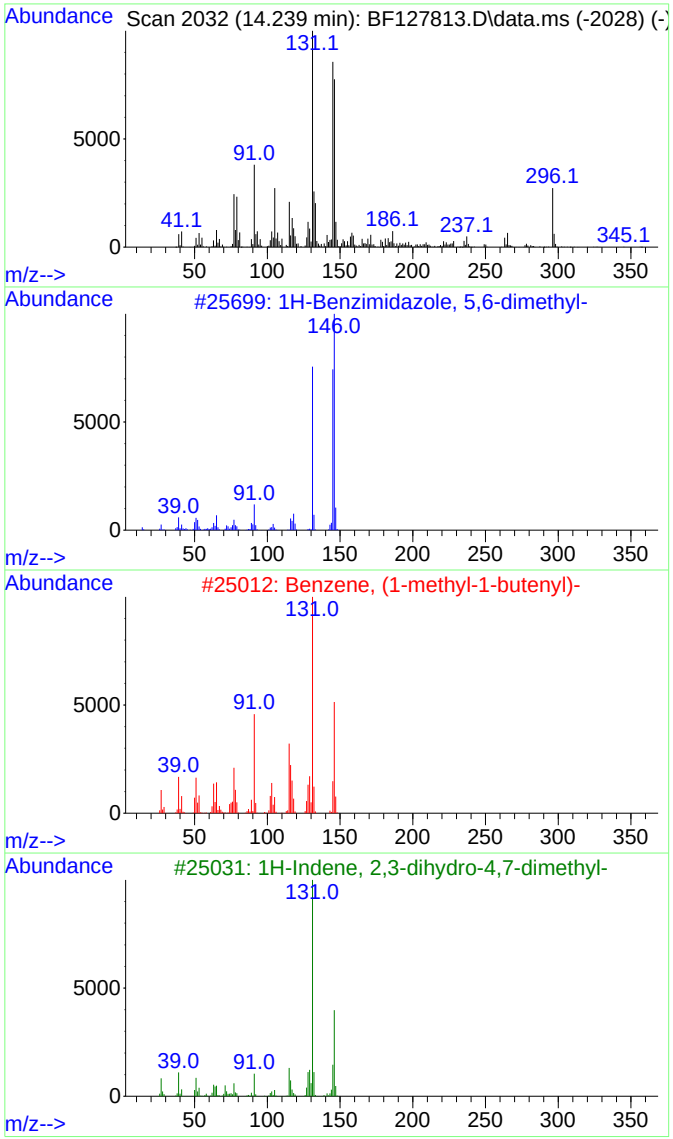
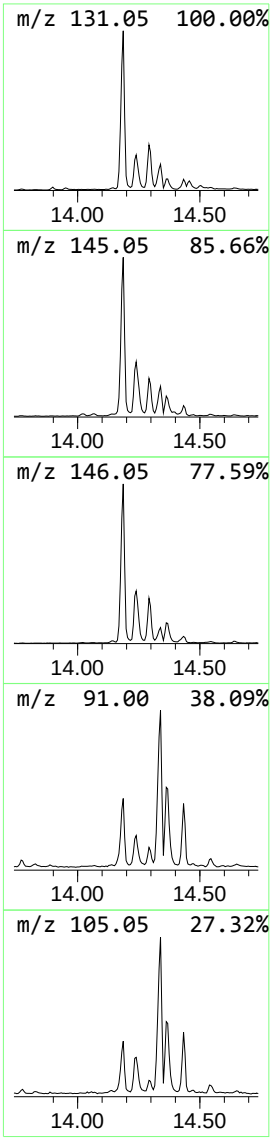
****
Peak Number 7 1H-Benzimidazole, 5,6-dimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.239	39.08 ng	1556620	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	58
2	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	55
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	49
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	49
5	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	49





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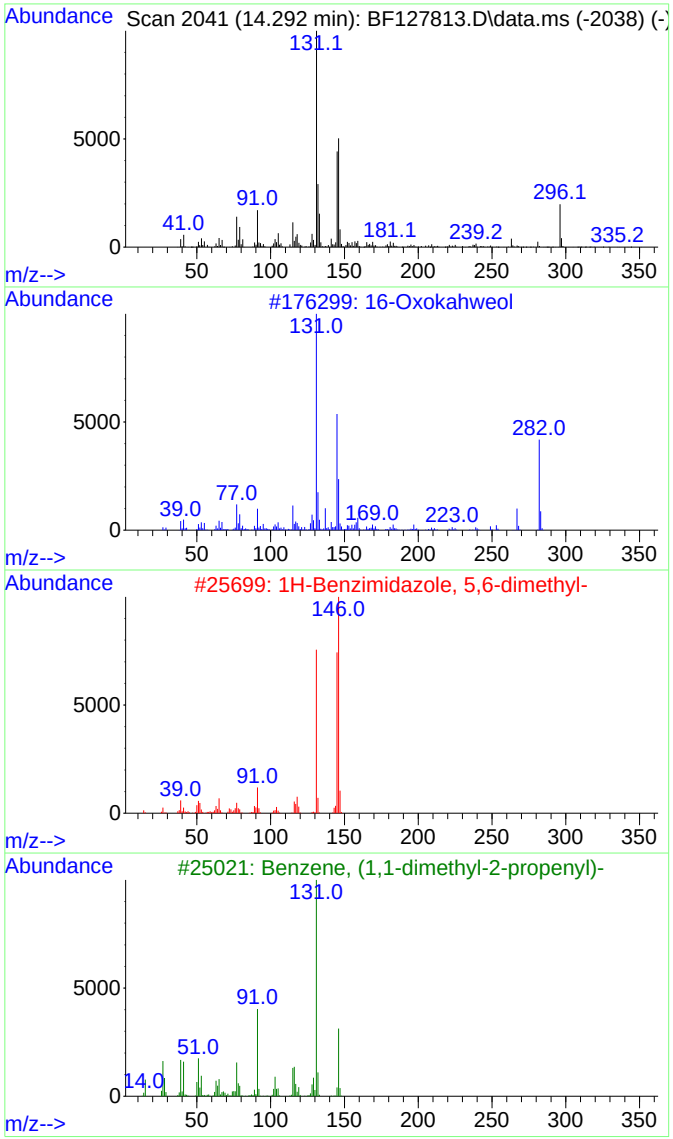
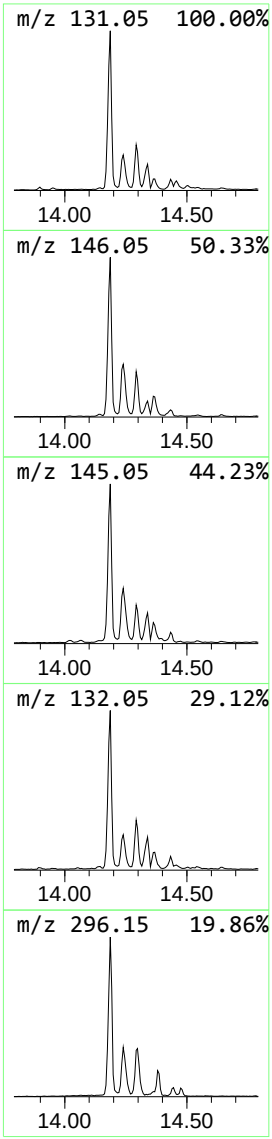
Peak Number 8 16-Oxokahweol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.292	24.60 ng	979972	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Oxokahweol	282	C19H22O2	108664-99-9	60
2	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	58
3	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	49
4	3-Phenyl-4,5-dimethyl-2,1-oxabor...	202	C13H19BO	1000062-26-1	47
5	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	46





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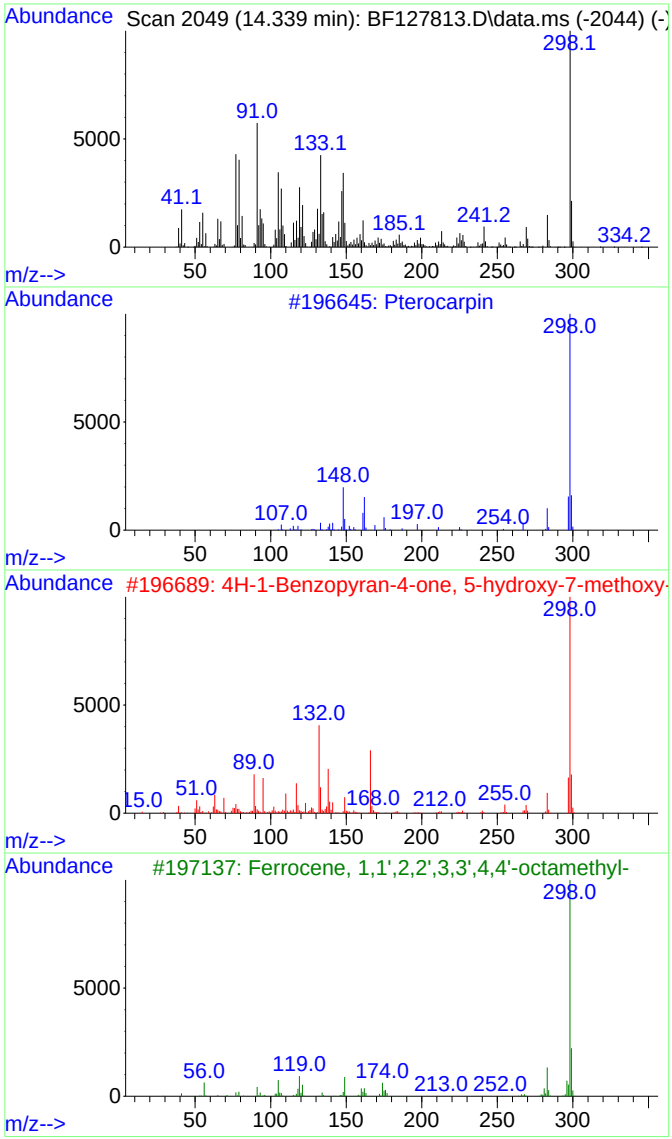
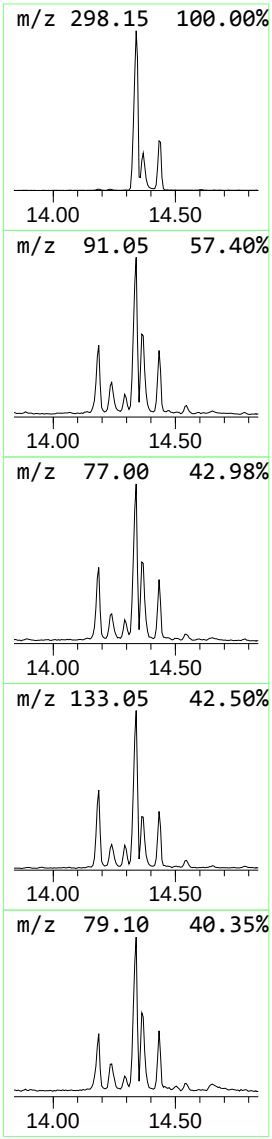
****

Peak Number 9 unknown14.339 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	140.43 ng	5593370	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pterocarpin	298	C17H14O5	000524-97-0	38
2	4H-1-Benzopyran-4-one, 5-hydroxy...	298	C17H14O5	034086-51-6	30
3	Ferrocene, 1,1',2,2',3,3',4,4'-o...	298	C18H26Fe	059568-28-4	30
4	6,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	093176-02-4	30
5	4H-1-Benzopyran-4-one, 2-(3,4-di...	298	C17H14O5	033513-36-9	30





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Data File : BF127813.D
Acq On : 15 Apr 2022 19:52
Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

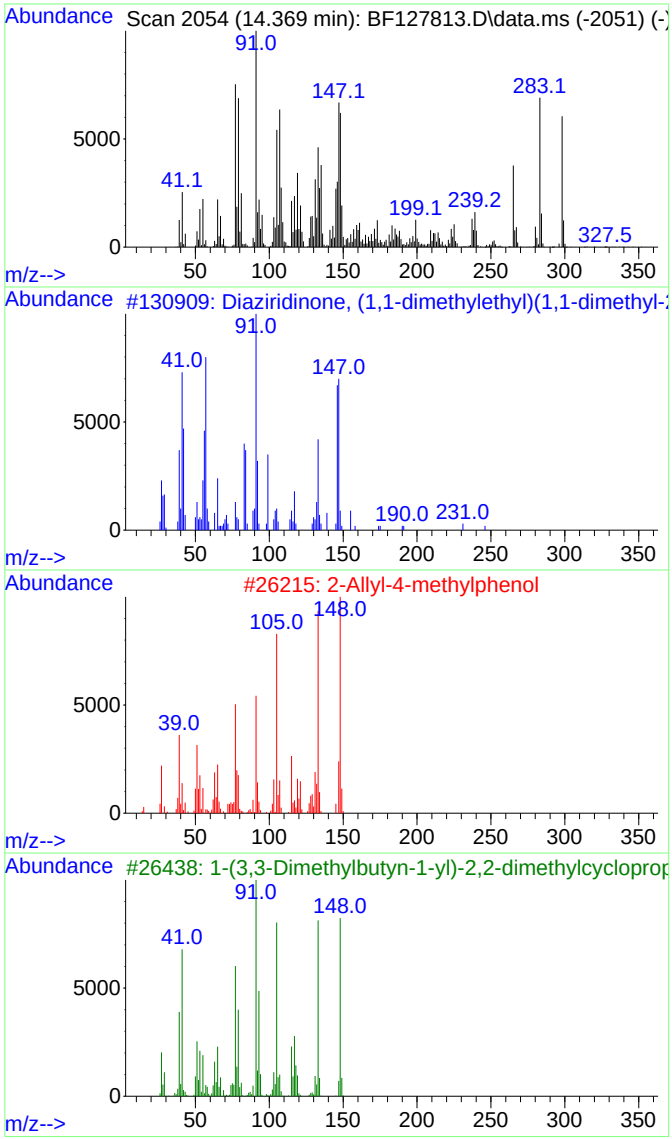
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

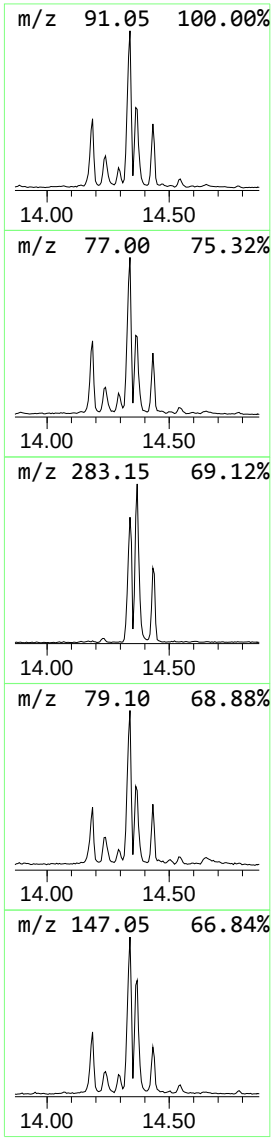
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Diaziridinone, (1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	77.22 ng	3075610	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diaziridinone, (1,1-dimethylethy...	246	C15H22N2O	019656-67-8	90
2	2-Allyl-4-methylphenol	148	C10H12O	006628-06-4	45
3	1-(3,3-Dimethylbutyn-1-yl)-2,2-d...	148	C11H16	1000222-04-6	41
4	Benzaldehyde, 2,4,5-trimethyl-	148	C10H12O	005779-72-6	38
5	1-Benzoxepin, 2,3,4,5-tetrahydro-	148	C10H12O	006169-78-4	25





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Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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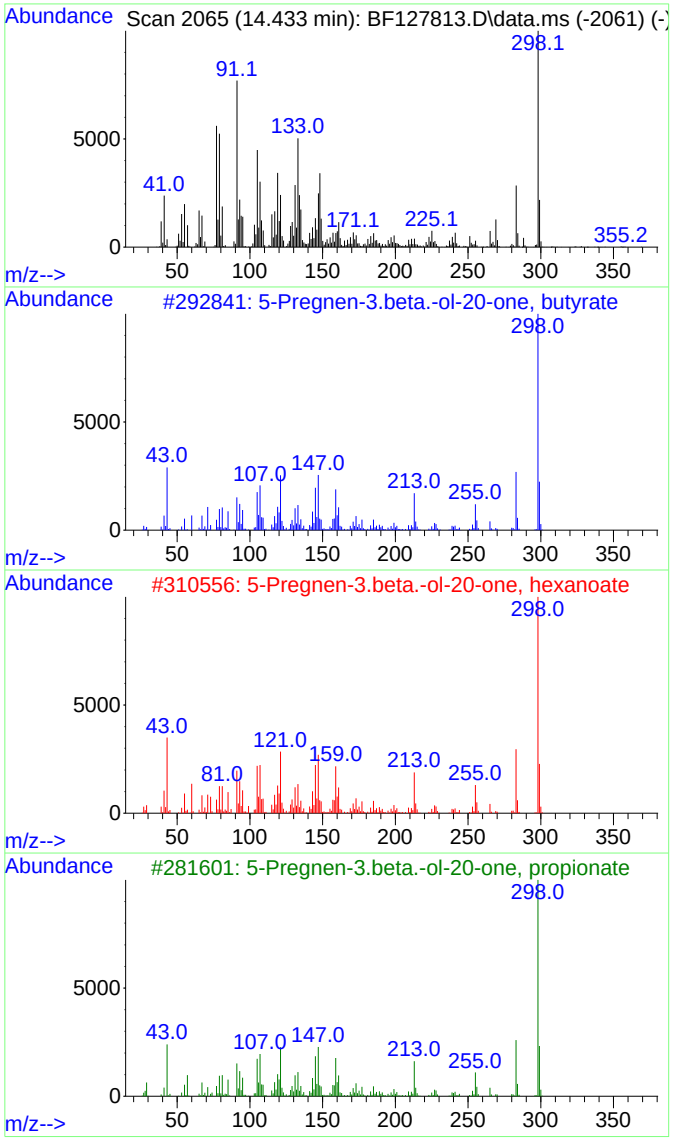
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

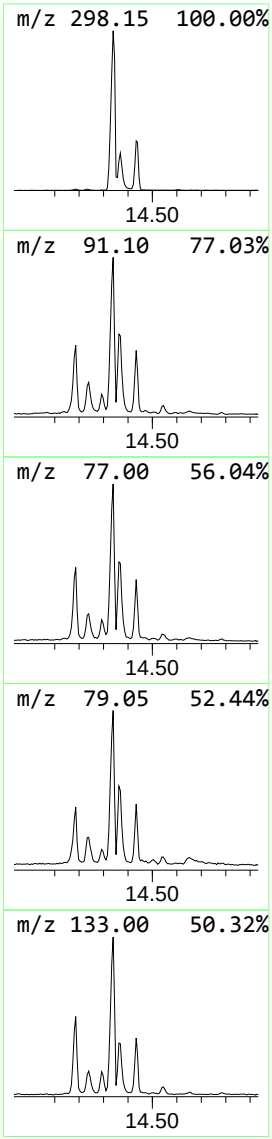
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 5-Pregnen-3.beta.-ol-20-one... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	51.70 ng	2059100	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Pregnen-3.beta.-ol-20-one, but...	386	C25H38O3	1000368-37-2	52
2	5-Pregnen-3.beta.-ol-20-one, hex...	414	C27H42O3	1000368-37-3	52
3	5-Pregnen-3.beta.-ol-20-one, pro...	372	C24H36O3	1000368-37-1	47
4	7,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	013198-99-7	42
5	(4Aalpha,18aalpha)-1,2,3,4,4a,9,...	298	C22H34	069651-19-0	42





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Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

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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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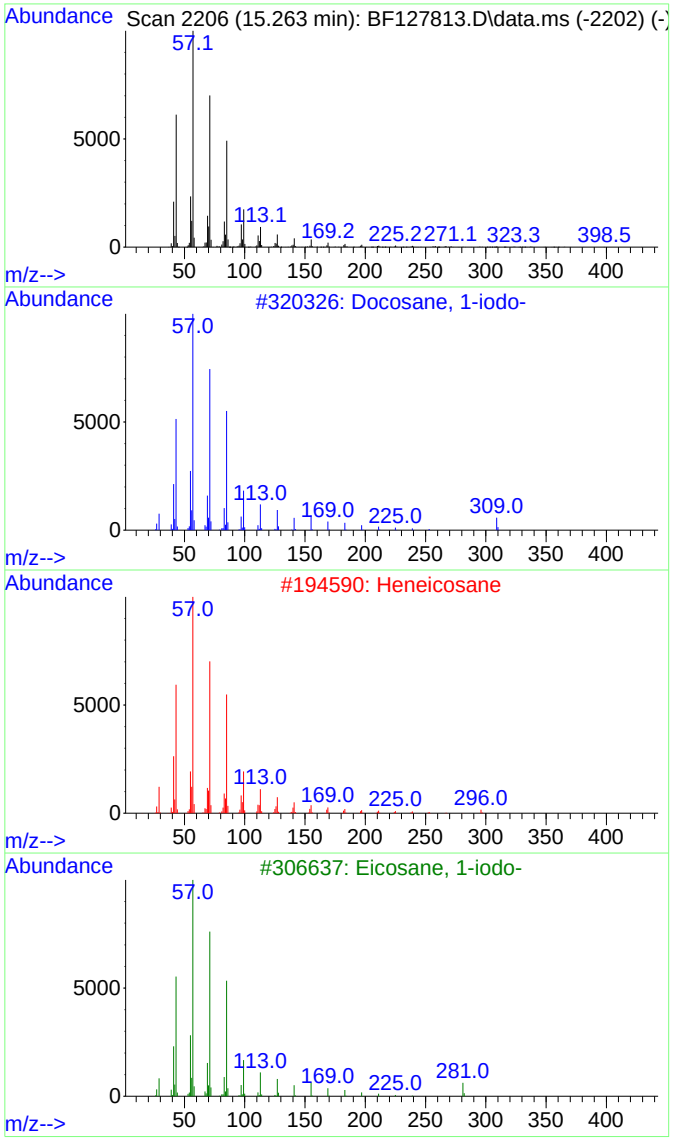
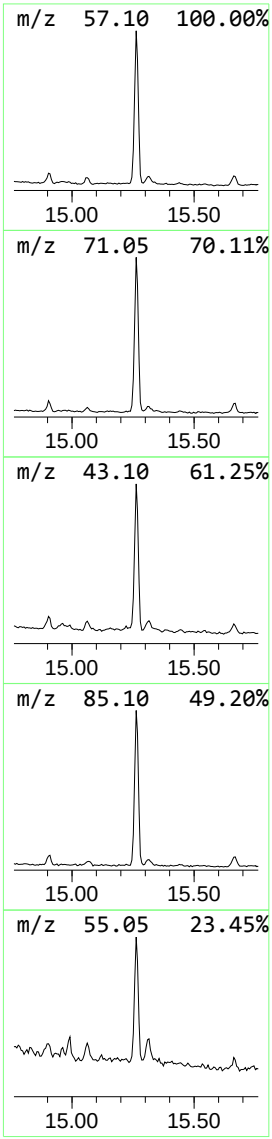
Peak Number 12 Docosane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.263	34.29 ng	1231120	Perylene-d12	15.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Octacosane	394	C28H58	000630-02-4	91





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Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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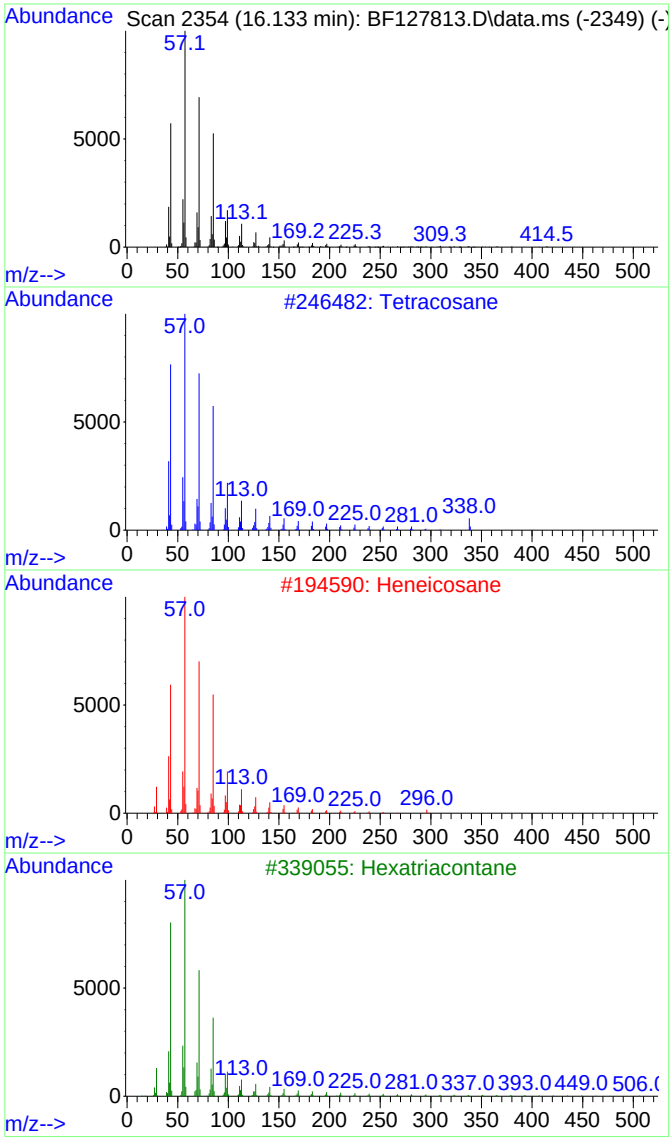
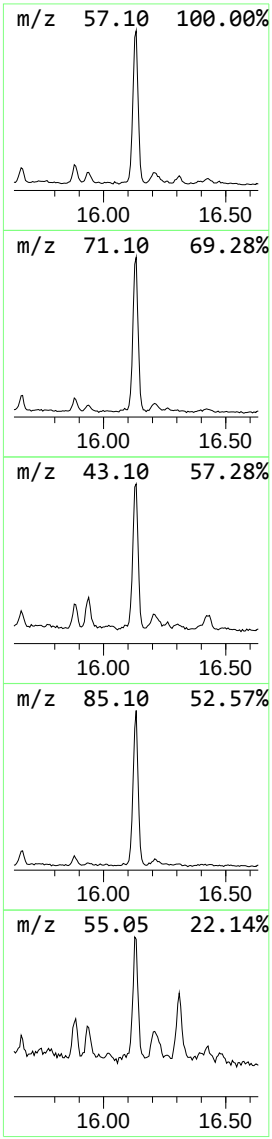
Peak Number 13 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	30.40 ng	1091660	Perylene-d12	15.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	1,3-Propanediol, ethyl tetracosy...	440	C29H60O2	1000406-35-7	91
5	Hexacosane	366	C26H54	000630-01-3	87





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Acq On : 15 Apr 2022 19:52
Operator : CG\JU
Sample : N2429-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-041422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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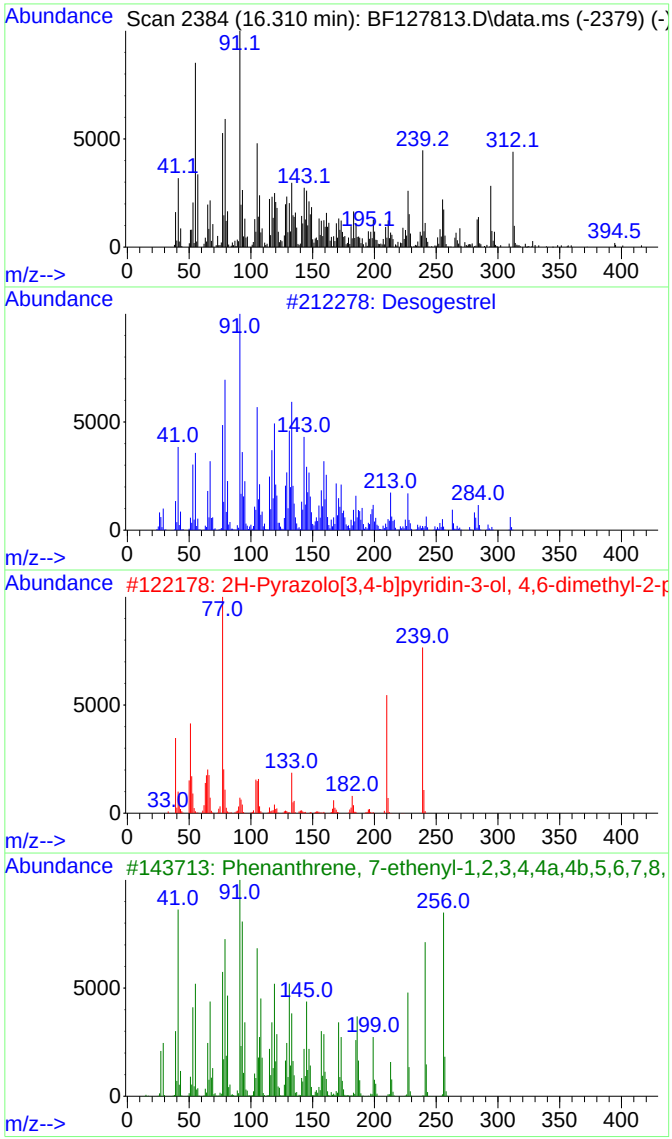
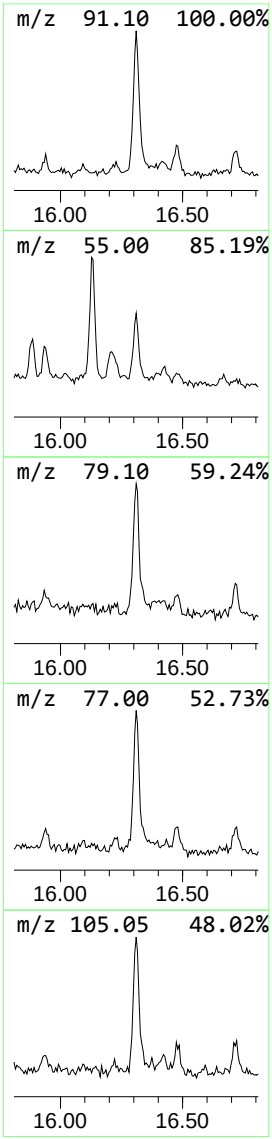
Peak Number 14 unknown16.310 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	19.26 ng	691717	Perylene-d12	15.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Desogestrel	310	C22H30O	054024-22-5	10
2	2H-Pyrazolo[3,4-b]pyridin-3-ol, ...	239	C14H13N3O	1000302-65-8	10
3	Phenanthrene, 7-ethenyl-1,2,3,4,...	256	C19H28	026549-04-2	9
4	Ethisterone	312	C21H28O2	000434-03-7	9
5	Bicyclo[3.1.1]hept-2-ene, 2,2'-(...	270	C20H30	057988-82-6	9





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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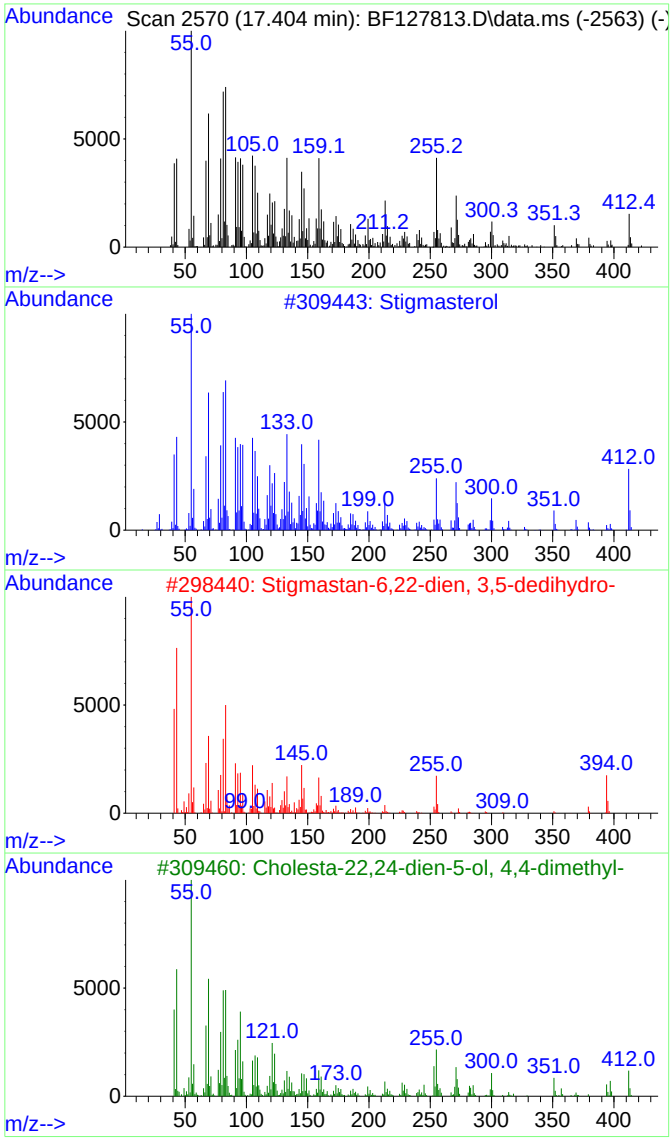
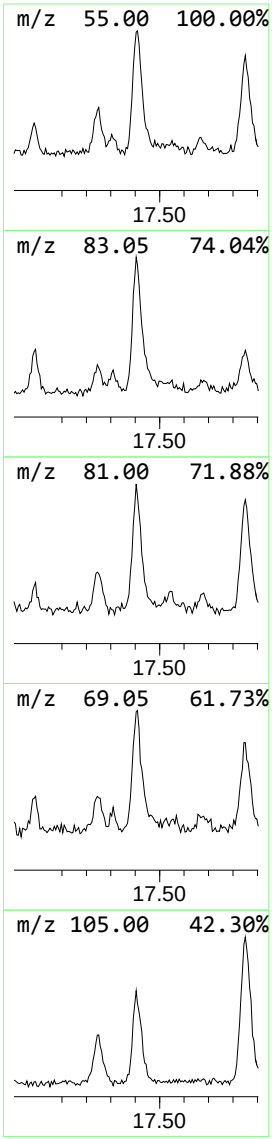
Peak Number 15 Stigmasterol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.404	36.23 ng	1301000	Perylene-d12	15.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	99
2	Stigmastan-6,22-dien, 3,5-dedihy...	394	C29H46	107304-12-1	91
3	Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	80
4	Cholesta-6,22,24-triene, 4,4-dim...	394	C29H46	1000128-66-9	49
5	Ergosta-5,22-dien-3-ol, (3.beta....	398	C28H46O	000474-67-9	30





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Operator : CG\JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-041422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
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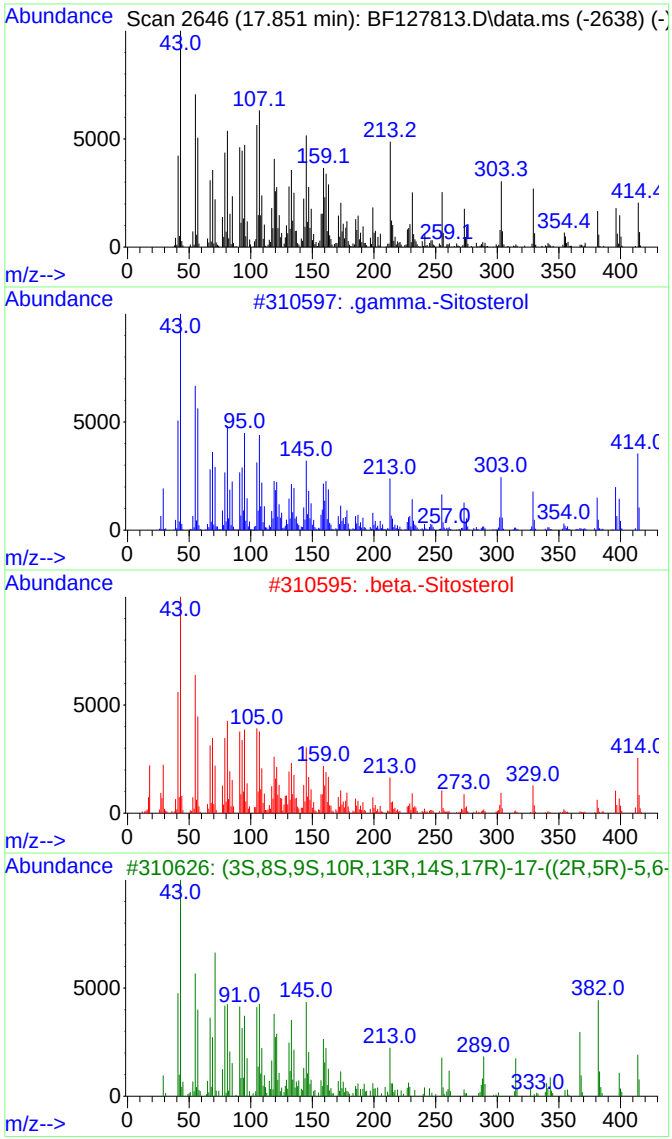
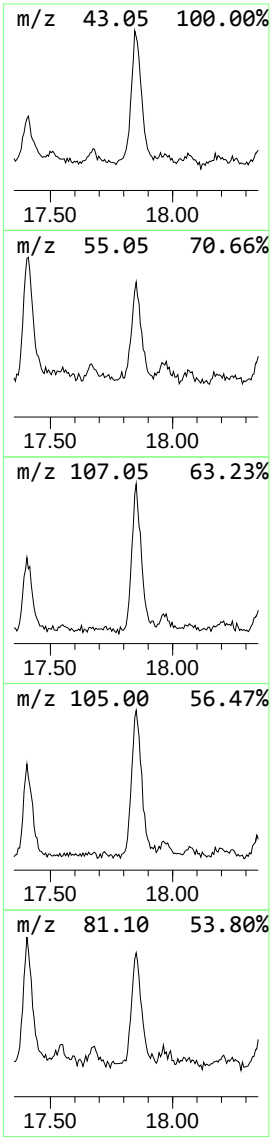
Peak Number 16 .gamma.-Sitosterol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.851	50.71 ng	1820860	Perylene-d12	15.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	94
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	60
4	Campesterol	400	C28H48O	000474-62-4	58
5	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	49





Tentatively Identified Compound (LSC) summary

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Acq On : 15 Apr 2022 19:52
Operator : CG\JU
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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
Hexadecanoic ac...	11.863	19.1	ng	800664	4	11.480	838934	20.0
n-Hexadecanoic ...	12.133	1608.5	ng	67473100	4	11.480	838934	20.0
9,12-Octadecadi...	12.557	61.5	ng	2579560	4	11.480	838934	20.0
16-Octadecenoic...	12.580	37.8	ng	1584160	4	11.480	838934	20.0
9,12-Octadecadi...	12.828	1619.5	ng	64503200	5	14.133	796598	20.0
Eicosanoic acid	13.545	100.2	ng	3991760	5	14.133	796598	20.0
1H-Benzimidazol...	14.239	39.1	ng	1556620	5	14.133	796598	20.0
16-Oxokahweol	14.292	24.6	ng	979972	5	14.133	796598	20.0
unknown14.339	14.339	140.4	ng	5593370	5	14.133	796598	20.0
Diaziridinone, ...	14.368	77.2	ng	3075610	5	14.133	796598	20.0
5-Pregnen-3.bet...	14.433	51.7	ng	2059100	5	14.133	796598	20.0
Docosane, 1-iodo-	15.263	34.3	ng	1231120	6	15.651	718112	20.0
Tetracosane	16.133	30.4	ng	1091660	6	15.651	718112	20.0
unknown16.310	16.310	19.3	ng	691717	6	15.651	718112	20.0
Stigmasterol	17.404	36.2	ng	1301000	6	15.651	718112	20.0
.gamma.-Sitosterol	17.851	50.7	ng	1820860	6	15.651	718112	20.0