LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035176.D
Acq On : 20 May 2022 14:56
Operator : CG/JU
Sample : N2872-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS001-1824-01

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_M\Methods\8270-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	401	407	419	rBV	1603801	2358883	4.32%	1.594%
2	7.075	669	678	687	rBV	1594570	2512613	4.60%	1.698%
3	7.904	811	819	828	rBV	441197	691219	1.27%	0.467%
4	9.063	1007	1016	1026	rBV	936040	1559996	2.86%	1.054%
5	10.704	1287	1295	1305	rBV	531915	913702	1.67%	0.618%
6	13.168	1707	1714	1728	rBV	2345401	3448657	6.31%	2.331%
7	14.539	1942	1947	1954	rBV	816265	1229607	2.25%	0.831%
8	15.362	2081	2087	2106	rVB	676050	1256434	2.30%	0.849%
9	15.915	2175	2181	2190	rVB2	470059	825162	1.51%	0.558%
10	16.027	2195	2200	2208	rBV	2122277	3040129	5.57%	2.055%
11	17.286	2409	2414	2426	rVB	1048416	1535890	2.81%	1.038%
12	18.221	2553	2573	2578	rBV	12959140	31564992	57.79%	21.334%
13	18.833	2670	2677	2680	rBV	352959	843257	1.54%	0.570%
14	19.274	2748	2752	2756	rBV	556830	772646	1.41%	0.522%
15	19.327	2756	2761	2764	rVV	1592105	2721735	4.98%	1.840%
16	19.356	2764	2766	2772	rVV2	1369530	2373996	4.35%	1.604%
17	19.503	2773	2791	2818	rVB	23057490	54620840	100.00%	36.916%
18	19.915	2855	2861	2864	rBV	4562780	5590623	10.24%	3.778%
19	19.950	2864	2867	2876	rVB	841450	1588043	2.91%	1.073%
20	20.809	3007	3013	3020	rVB	1345884	2343478	4.29%	1.584%
21	21.468	3121	3125	3129	rBV	1368932	1804042	3.30%	1.219%
22	21.527	3129	3135	3142	rVB	1811384	3275641	6.00%	2.214%
23	22.244	3251	3257	3271	rBV	2198299	3881214	7.11%	2.623%
24	23.038	3385	3392	3401	rBV	1439105	3450204	6.32%	2.332%
25	23.144	3404	3410	3424	rVB	623198	1461985	2.68%	0.988%
26	23.856	3525	3531	3538	rBV2	992137	2026816	3.71%	1.370%
27	23.950	3541	3547	3555	rVB	838713	2196172	4.02%	1.484%
28	24.974	3715	3721	3731	rVB	535656	1455323	2.66%	0.984%
29	25.844	3859	3869	3888	rVB2	1955206	6616107	12.11%	4.472%

Sum of corrected areas: 147959406

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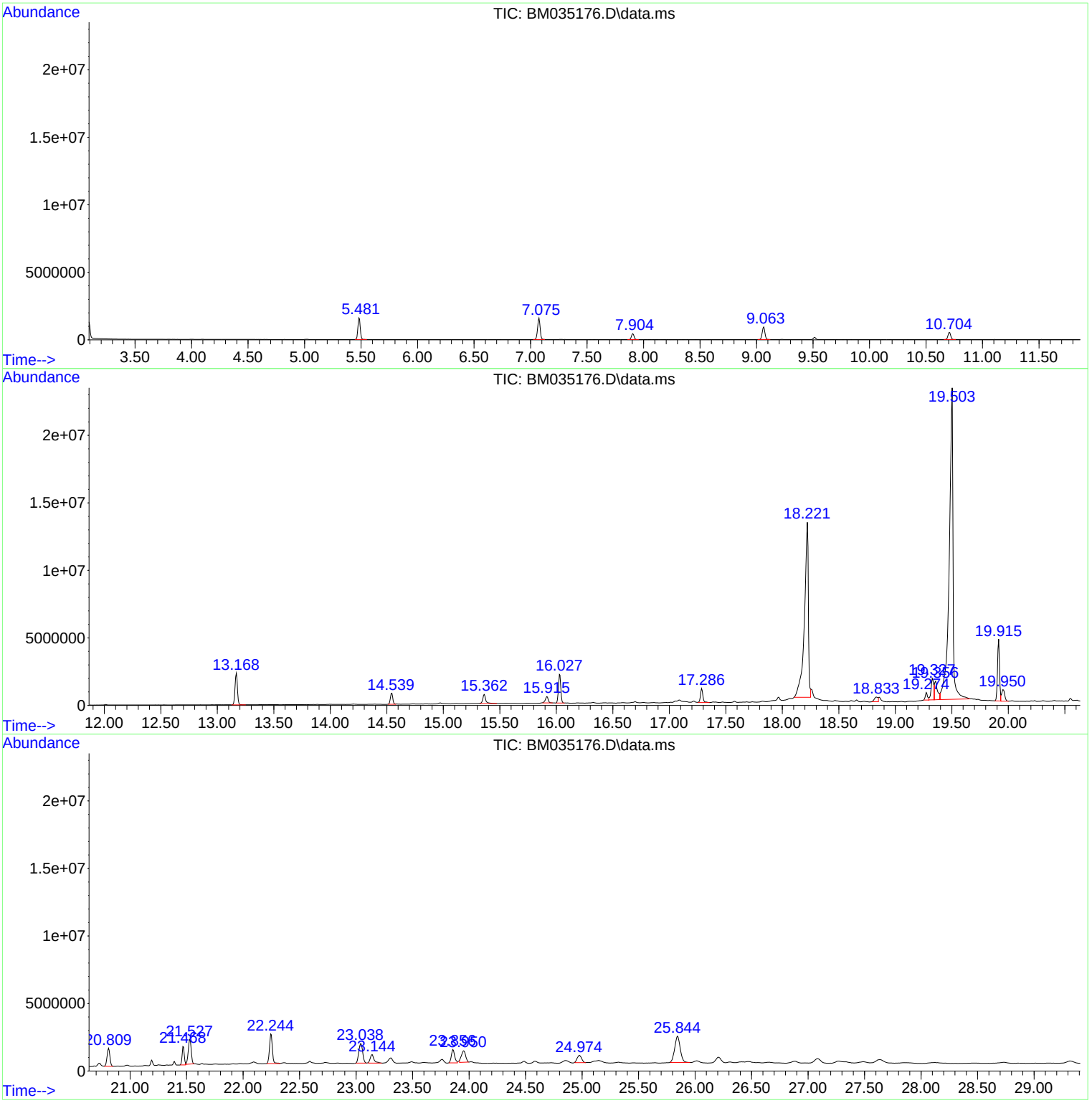
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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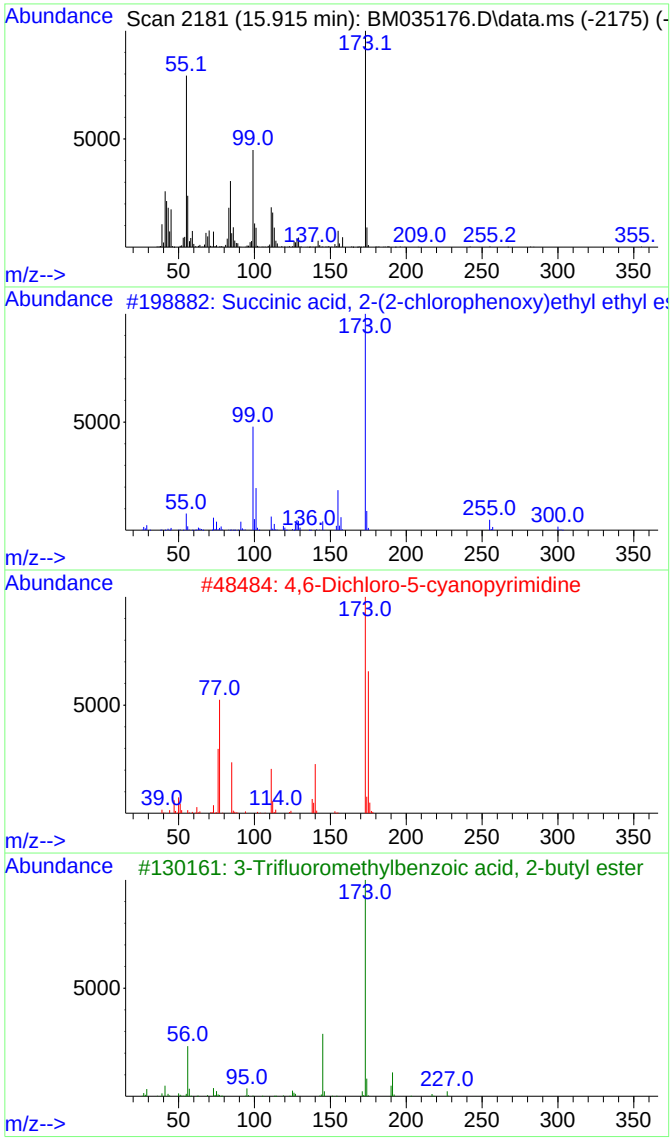
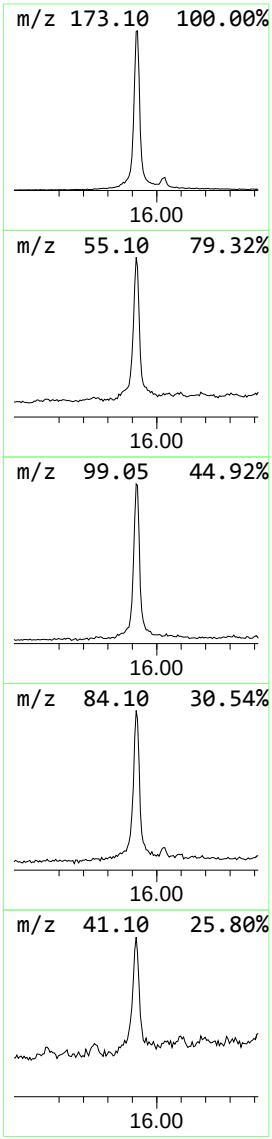
Peak Number 1 unknown15.915 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	13.42 ng	825162	Acenaphthene-d10	14.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-(2-chlorophenox...	300	C14H17ClO5	1000381-53-1	38
2	4,6-Dichloro-5-cyanopyrimidine	173	C5HCl2N3	005305-45-3	35
3	3-Trifluoromethylbenzoic acid, 2...	246	C12H13F3O2	1000282-68-1	32
4	3-Trifluoromethylbenzoic acid, 2...	274	C14H17F3O2	1000355-14-0	28
5	2-Trifluoromethylbenzoic acid, 2...	302	C16H21F3O2	1000282-64-8	25





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ClientSampleId :
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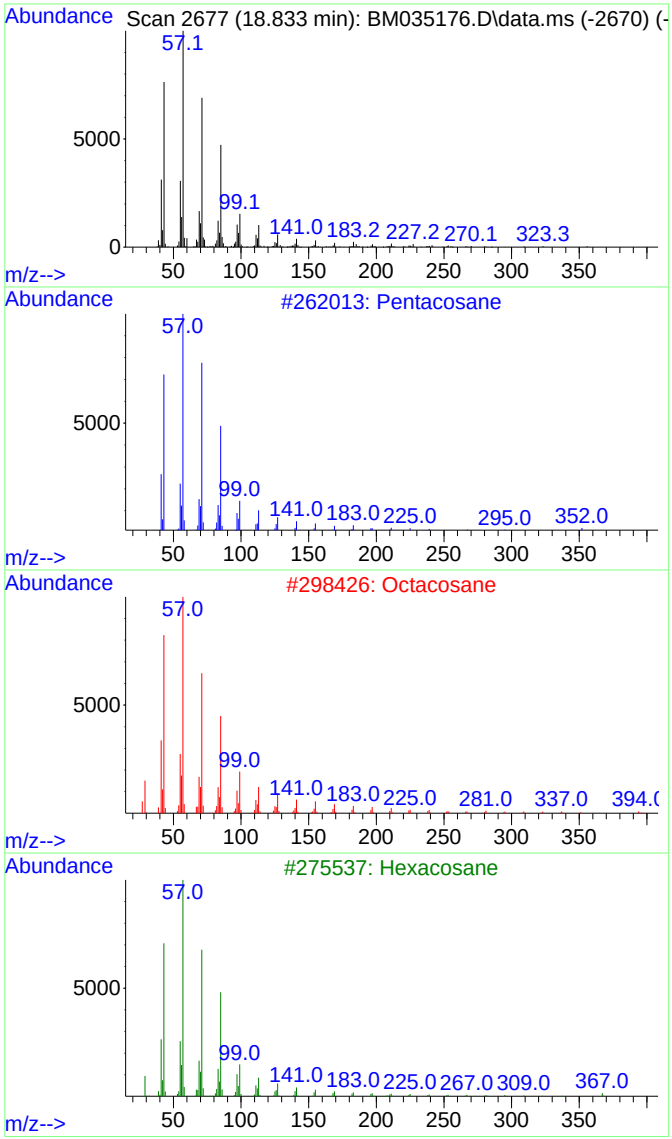
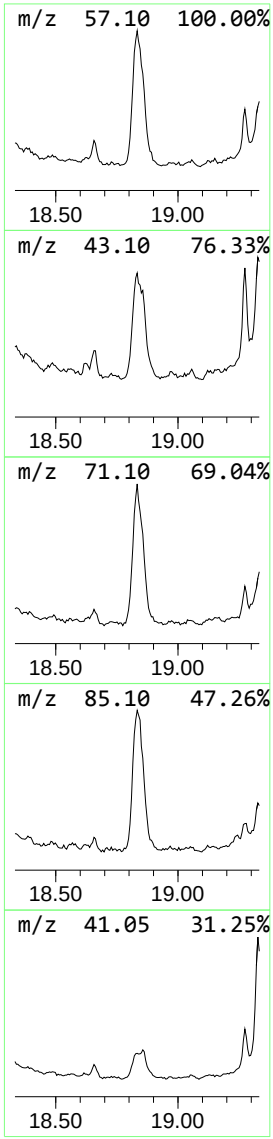
Peak Number 2 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.833	10.98 ng	843257	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
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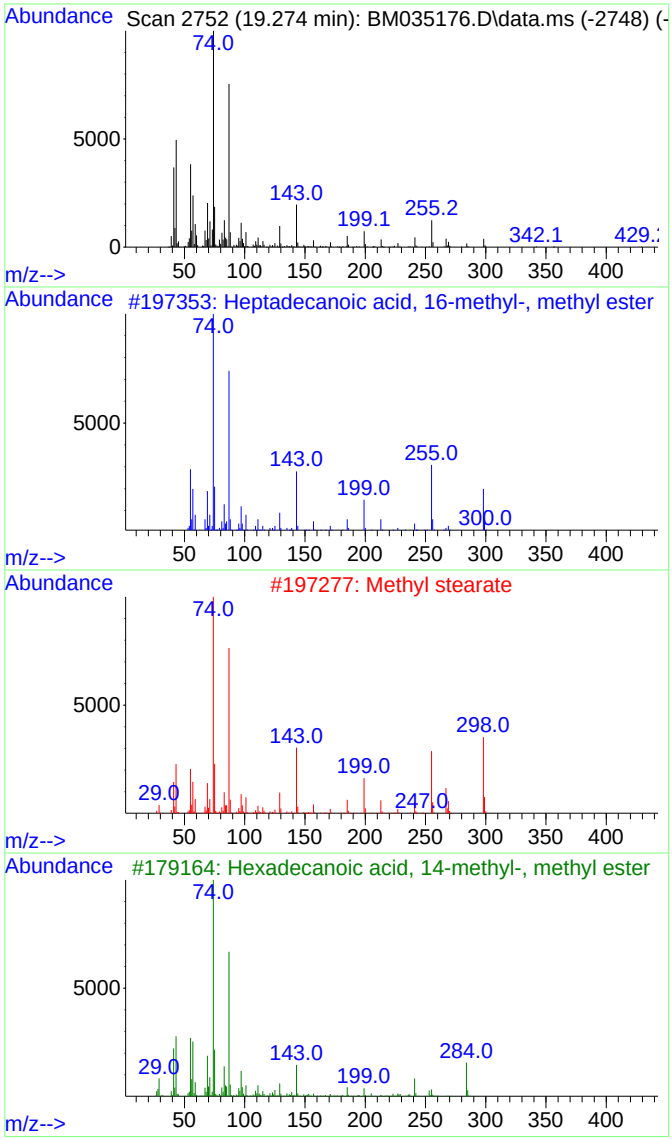
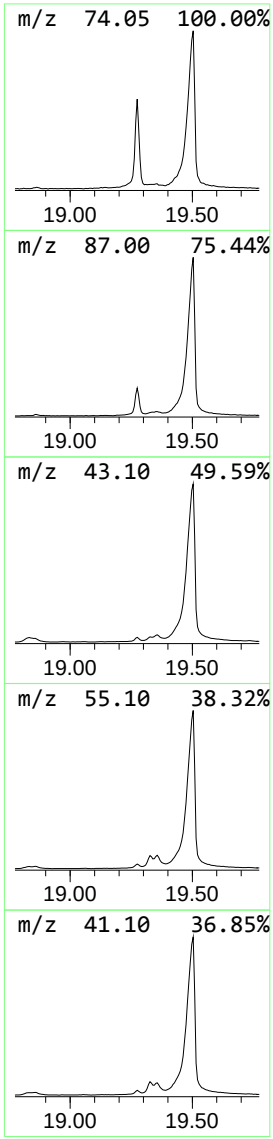
****
Peak Number 3 Heptadecanoic acid, 16-meth... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	10.06 ng	772646	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	99
2	Methyl stearate	298	C19H38O2	000112-61-8	98
3	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	96
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	95
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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P022-SS001-1824-01

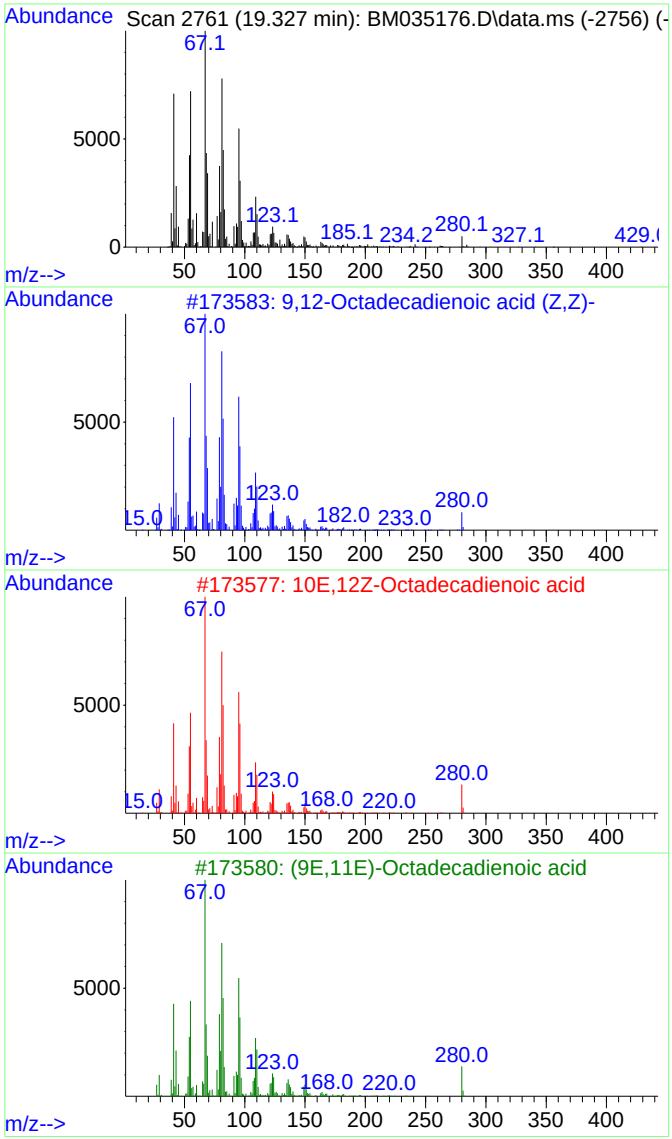
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

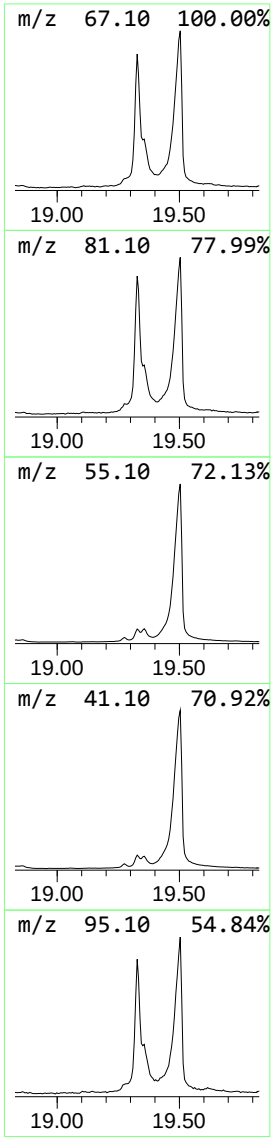
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.327	35.44 ng	2721740	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
3	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
4	Linoelaidic acid	280	C18H32O2	000506-21-8	96
5	7-Hexadecyne	222	C16H30	074685-28-2	91





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Instrument :
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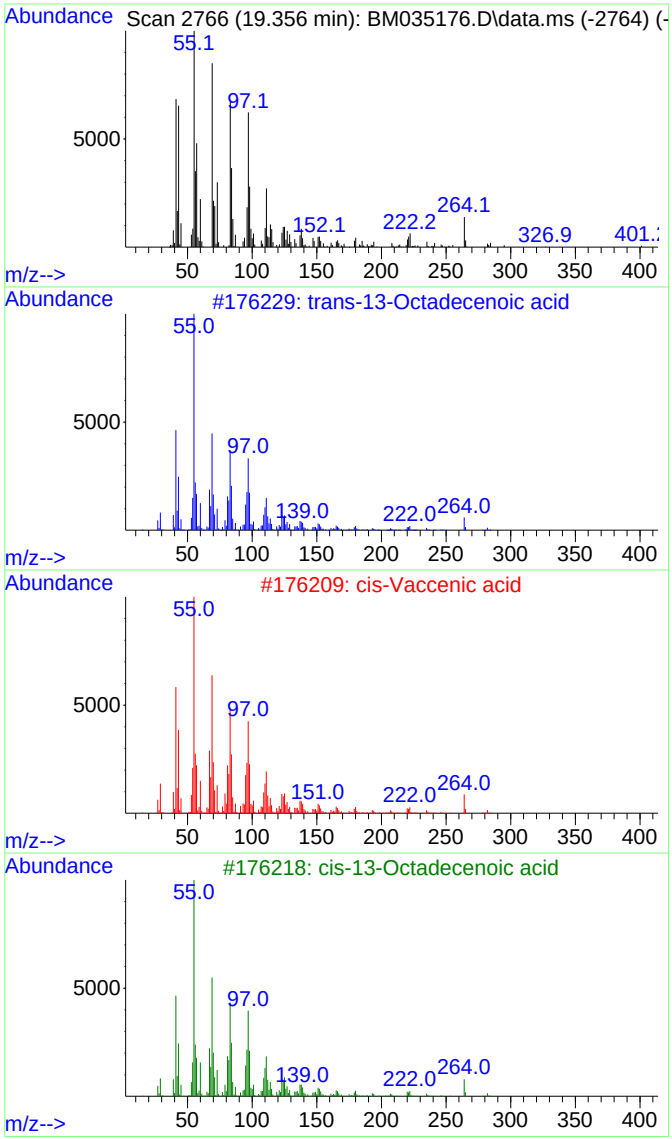
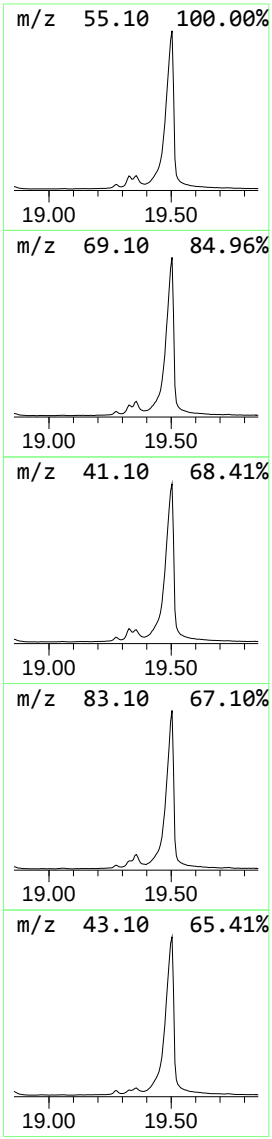
Peak Number 5 trans-13-Octadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.356	30.91 ng	2374000	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	83
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	83
4	1-Dodecanol	186	C12H26O	000112-53-8	59
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	46





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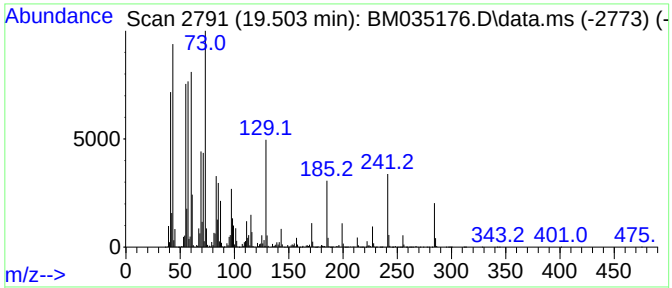
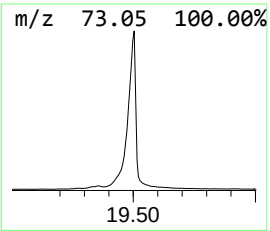
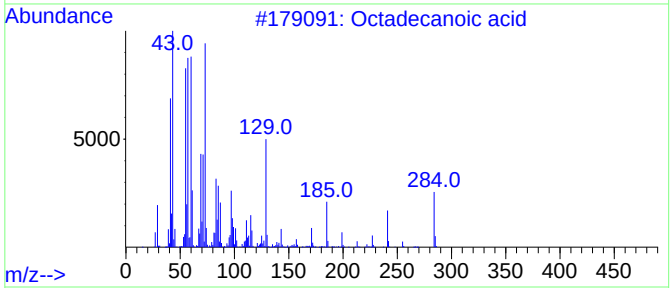
Peak Number 6 Octadecanoic acid Concentration Rank 1

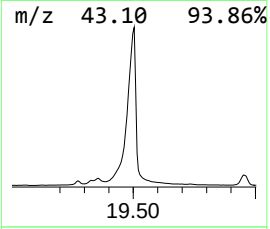
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.503	605.54 ng	54620800	Chrysene-d12	21.468

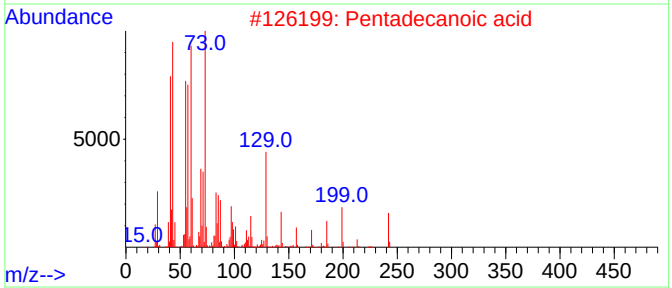
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62

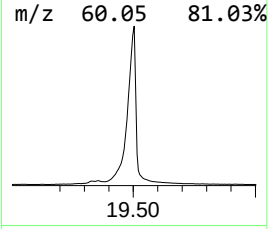


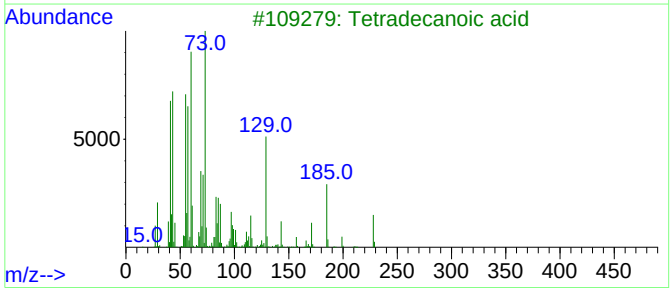


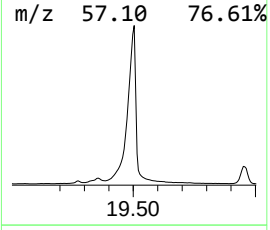


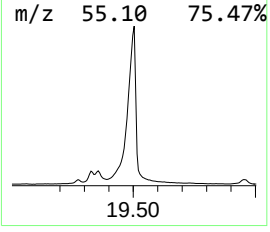












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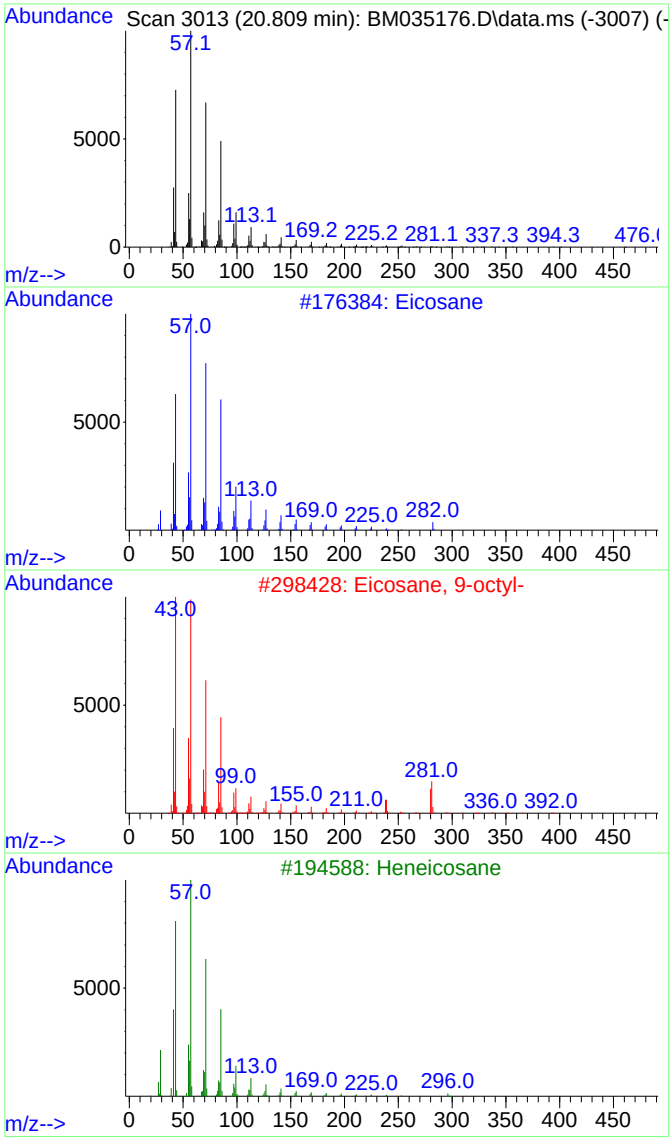
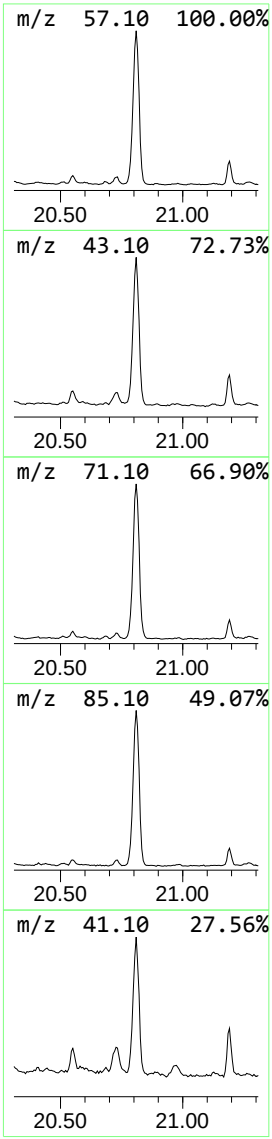
****

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	25.98 ng	2343480	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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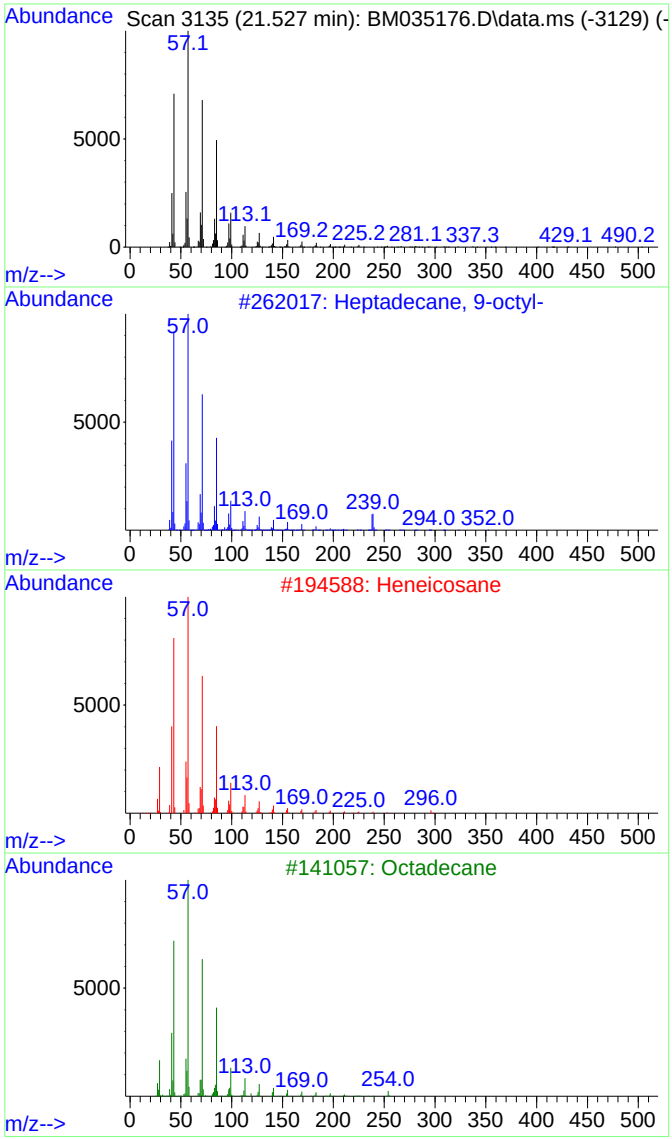
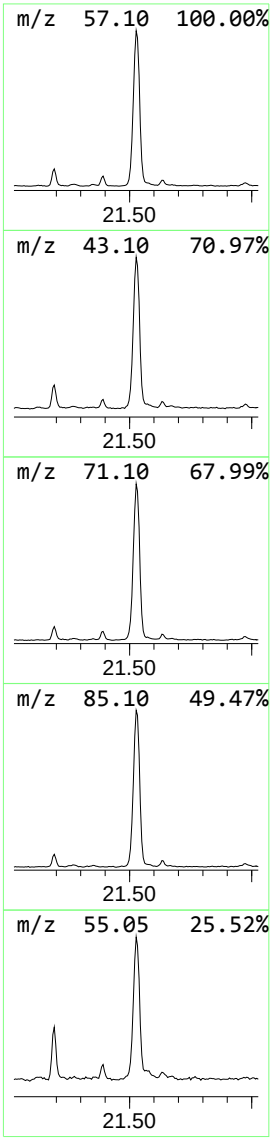
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.527	36.31 ng	3275640	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	99
2	Heneicosane	296	C21H44	000629-94-7	97
3	Octadecane	254	C18H38	000593-45-3	95
4	Eicosane	282	C20H42	000112-95-8	95
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035176.D
Acq On : 20 May 2022 14:56
Operator : CG/JU
Sample : N2872-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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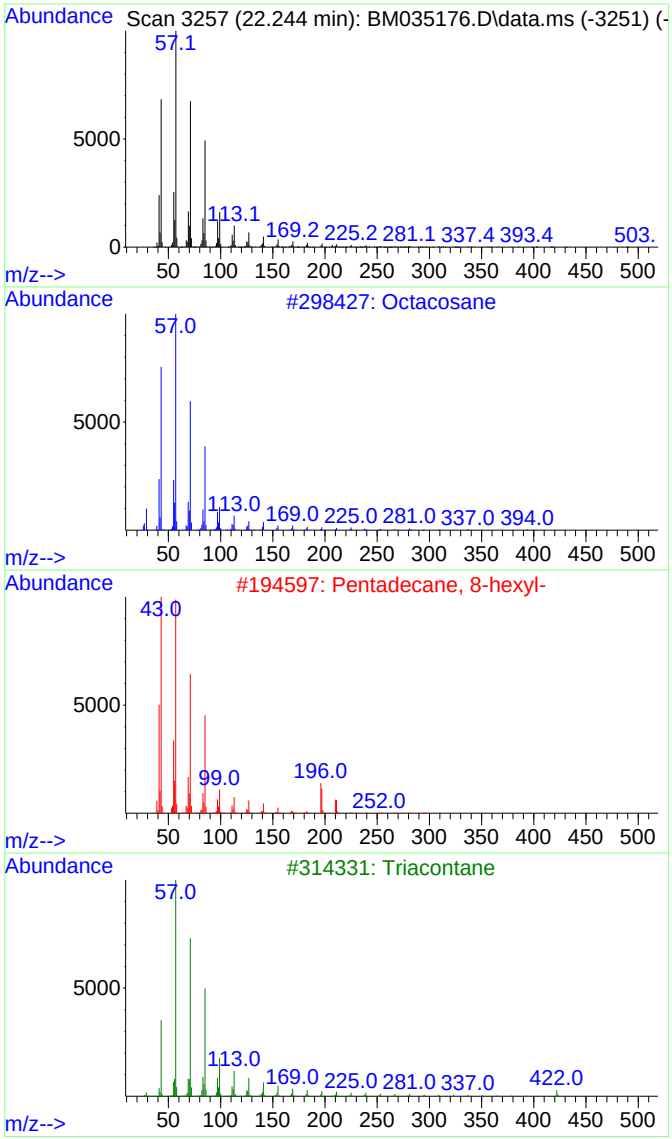
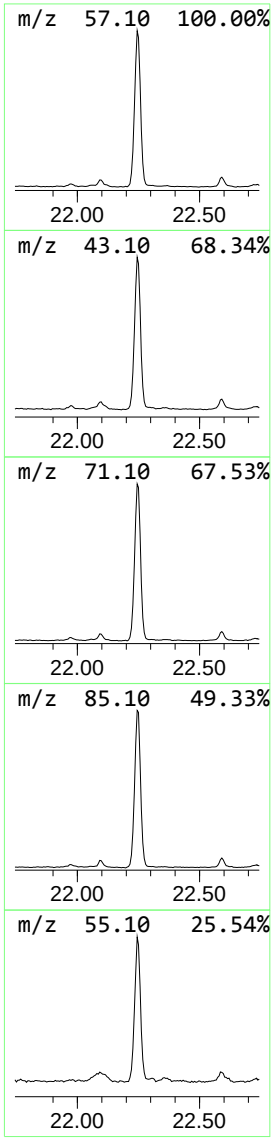
Peak Number 9 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.244	43.03 ng	3881210	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	96
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3	Triacontane	422	C30H62	000638-68-6	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Sample : N2872-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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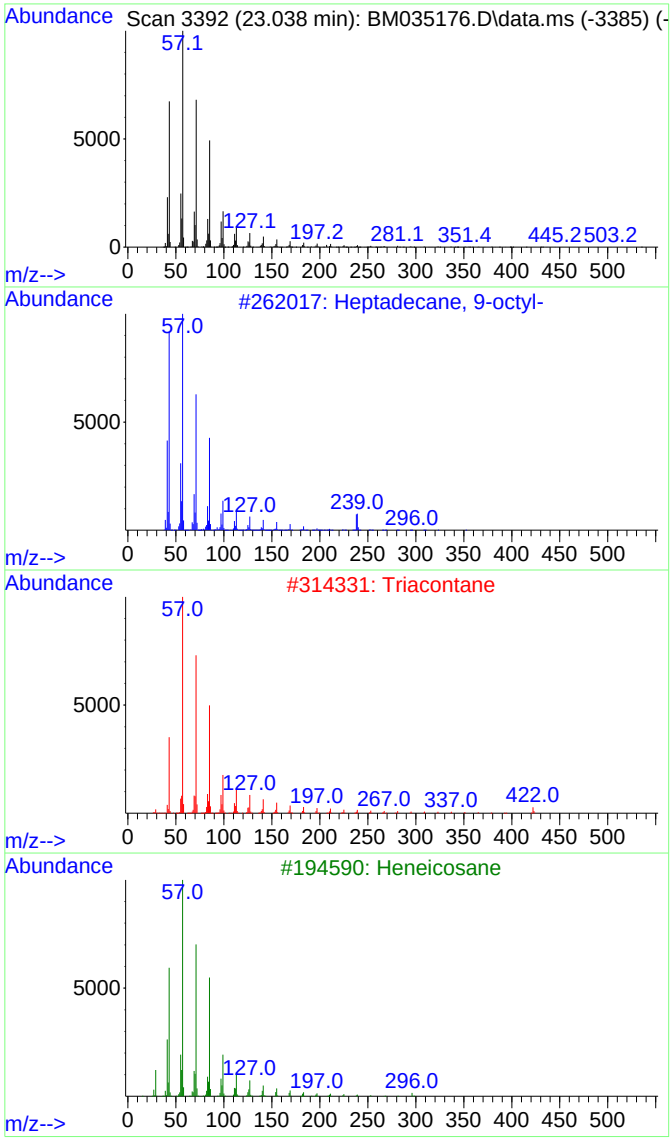
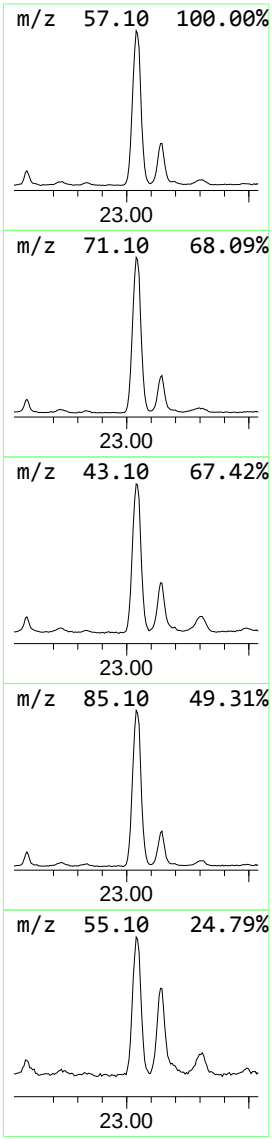
Peak Number 10 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.038	34.05 ng	3450200	Perylene-d12	23.856

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Triacontane	422	C30H62	000638-68-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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Sample : N2872-13
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P022-SS001-1824-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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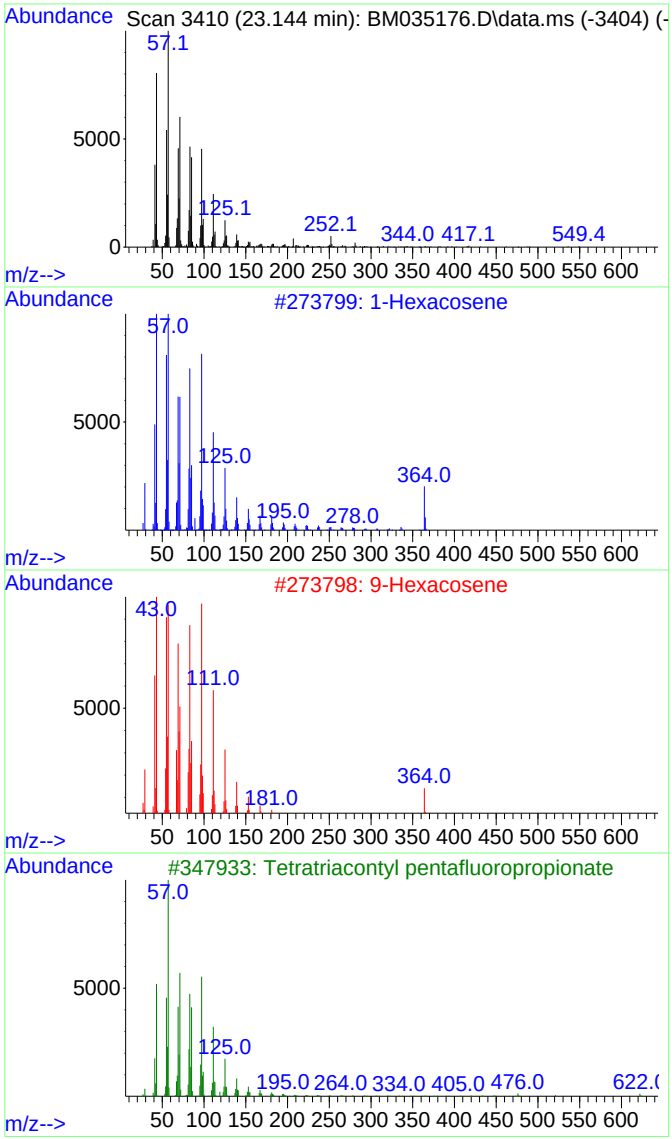
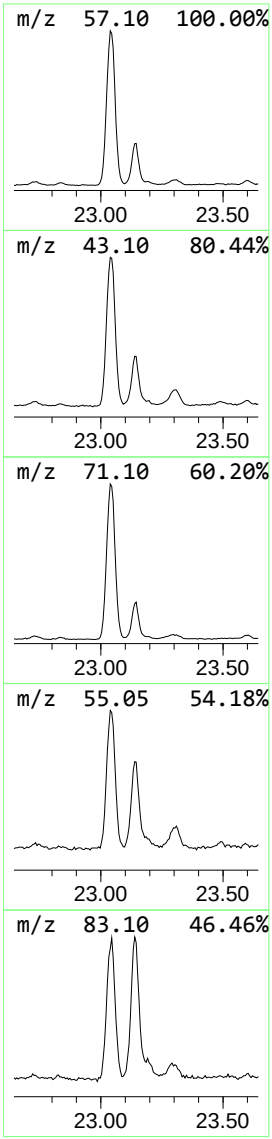
Peak Number 11 1-Hexacosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.144	14.43 ng	1461990	Perylene-d12	23.856

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	96
2	9-Hexacosene	364	C26H52	071502-22-2	93
3	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
4	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
5	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91





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Acq On : 20 May 2022 14:56
Operator : CG/JU
Sample : N2872-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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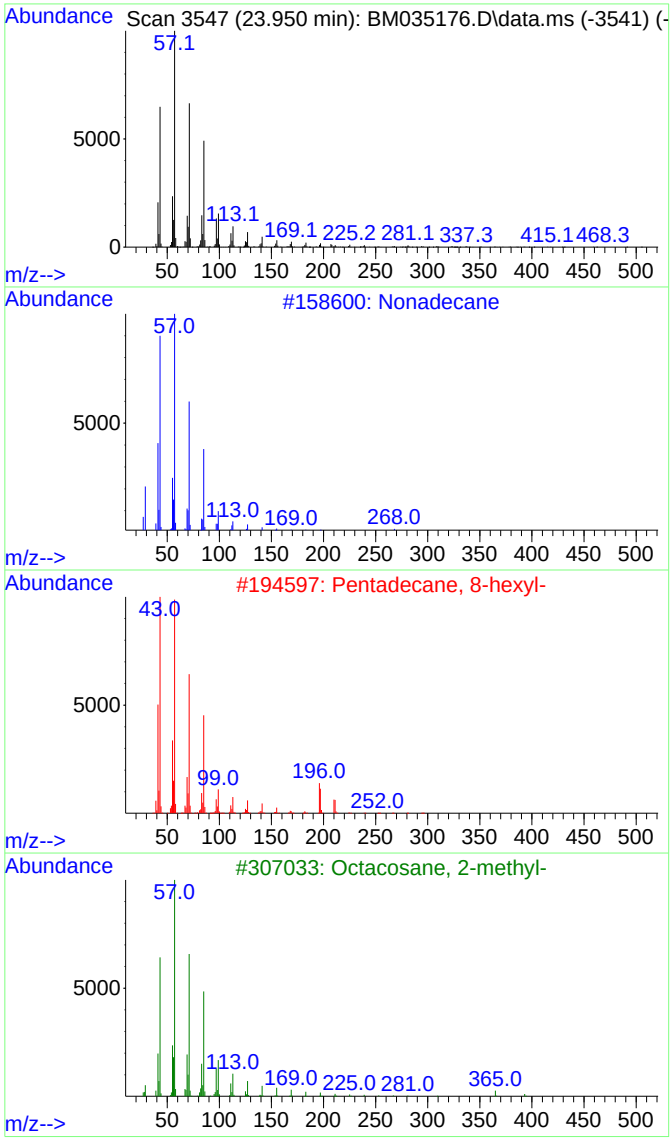
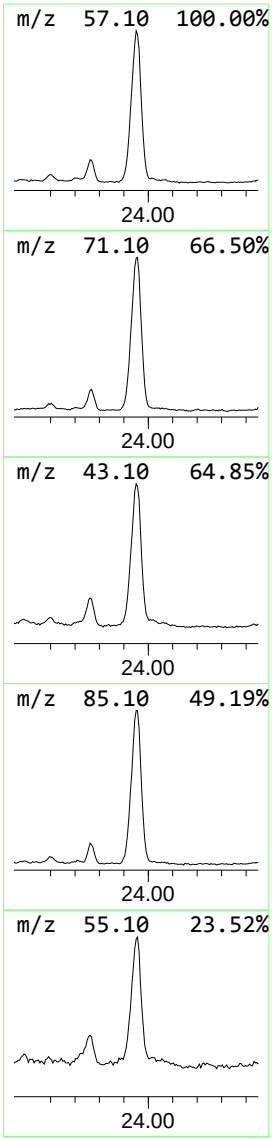
Peak Number 12 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.950	21.67 ng	2196170	Perylene-d12	23.856

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91





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Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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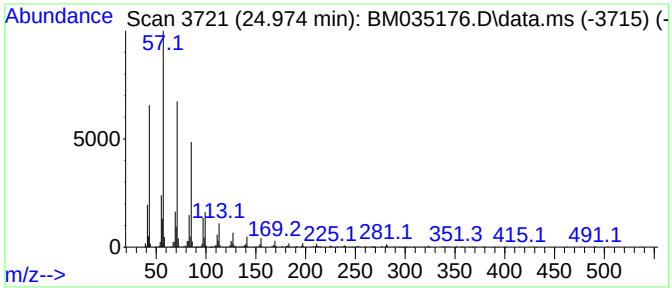
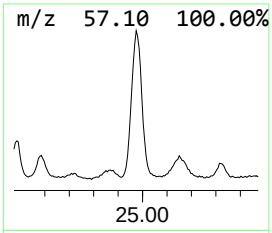
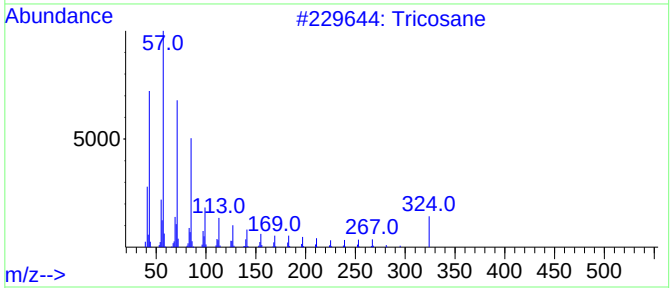
Peak Number 13 Tricosane Concentration Rank 11

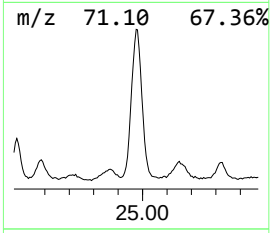
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.974	14.36 ng	1455320	Perylene-d12	23.856

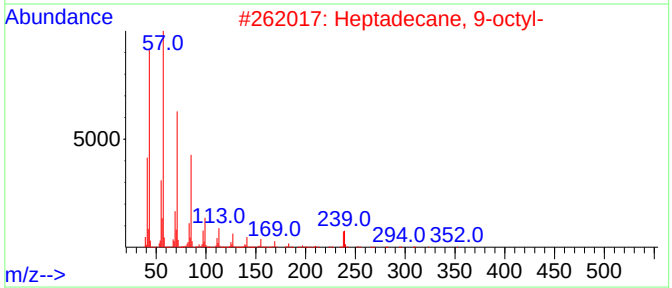
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
4	2-Methylpentacosane	366	C26H54	000629-87-8	95
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	91

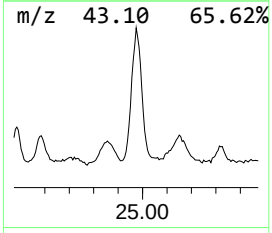


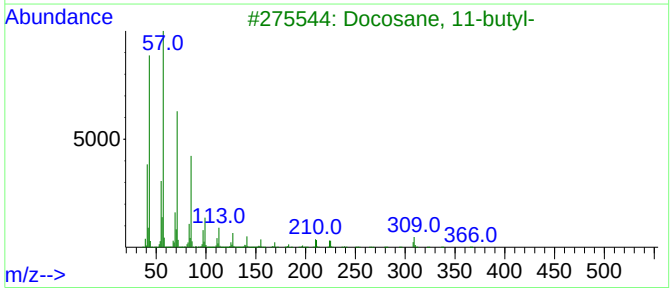


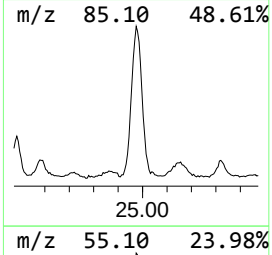


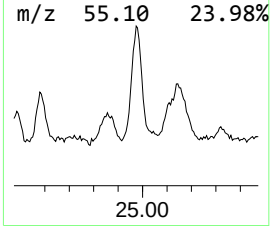












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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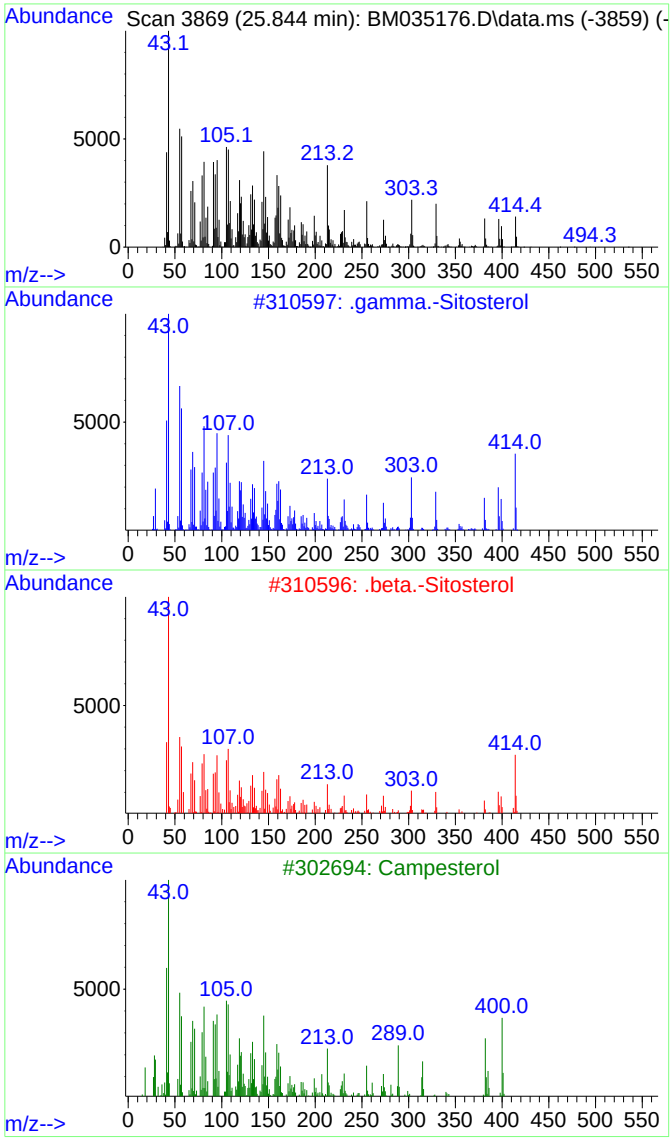
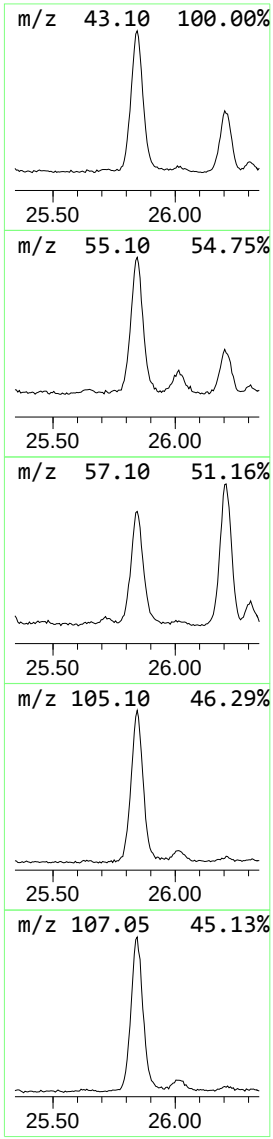
Peak Number 14 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.844	65.29 ng	6616110	Perylene-d12	23.856

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	95
3	Campesterol	400	C28H48O	000474-62-4	49
4	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	38
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	35





Tentatively Identified Compound (LSC) summary

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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
unknown15.915	15.915	13.4	ng	825162	3	14.545	1229610	20.0
Pentacosane	18.833	11.0	ng	843257	4	17.286	1535890	20.0
Heptadecanoic a...	19.274	10.1	ng	772646	4	17.286	1535890	20.0
9,12-Octadecadi...	19.327	35.4	ng	2721740	4	17.286	1535890	20.0
trans-13-Octade...	19.356	30.9	ng	2374000	4	17.286	1535890	20.0
Octadecanoic acid	19.503	605.5	ng	54620800	5	21.468	1804040	20.0
Eicosane	20.809	26.0	ng	2343480	5	21.468	1804040	20.0
Heptadecane, 9-...	21.527	36.3	ng	3275640	5	21.468	1804040	20.0
Octacosane	22.244	43.0	ng	3881210	5	21.468	1804040	20.0
Triacontane	23.038	34.0	ng	3450200	6	23.856	2026820	20.0
1-Hexacosene	23.144	14.4	ng	1461990	6	23.856	2026820	20.0
Nonadecane	23.950	21.7	ng	2196170	6	23.856	2026820	20.0
Tricosane	24.974	14.4	ng	1455320	6	23.856	2026820	20.0
.gamma.-Sitosterol	25.844	65.3	ng	6616110	6	23.856	2026820	20.0