LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037286.D
Acq On : 31 Oct 2022 12:40
Operator : CG/JU
Sample : N5318-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221107-COMP-06

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-BM102822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	315	321	329	rBV	631058	841722	4.63%	0.743%
2	5.440	393	400	412	rBV	4124291	5672448	31.22%	5.010%
3	7.045	666	673	686	rBV	3844119	5963748	32.83%	5.268%
4	7.869	805	813	821	rBV	1010659	1582974	8.71%	1.398%
5	9.034	1004	1011	1019	rBV	2173297	3578542	19.70%	3.161%
6	10.451	1246	1252	1264	rBV	256651	451314	2.48%	0.399%
7	10.669	1282	1289	1296	rBV	1364991	2194214	12.08%	1.938%
8	13.127	1701	1707	1714	rBV	5204522	7302485	40.20%	6.450%
9	13.986	1848	1853	1859	rVB	125781	214323	1.18%	0.189%
10	14.504	1935	1941	1948	rVB	1895580	2692291	14.82%	2.378%
11	14.927	2009	2013	2021	rVB3	225831	478654	2.63%	0.423%
12	15.992	2189	2194	2206	rVB2	5040079	7479798	41.17%	6.607%
13	16.645	2302	2305	2309	rBV4	127344	190670	1.05%	0.168%
14	17.245	2402	2407	2413	rBV	2178459	2977749	16.39%	2.630%
15	17.815	2497	2504	2517	rVB3	561884	2265221	12.47%	2.001%
16	18.139	2554	2559	2573	rVB	2495712	3528307	19.42%	3.116%
17	18.474	2613	2616	2626	rVB3	238770	392070	2.16%	0.346%
18	18.903	2681	2689	2702	rVB2	1810721	4798831	26.41%	4.239%
19	19.268	2748	2751	2753	rBV2	221679	300044	1.65%	0.265%
20	19.415	2771	2776	2785	rVB	2318911	3148534	17.33%	2.781%
21	19.580	2798	2804	2815	rVB2	1520903	3279278	18.05%	2.896%
22	19.862	2841	2852	2861	rBV2	11131165	18167457	100.00%	16.047%
23	20.174	2901	2905	2913	rVB	622371	909220	5.00%	0.803%
24	20.656	2980	2987	2994	rBV	1990088	3767856	20.74%	3.328%
25	21.097	3058	3062	3064	rBV4	368704	560613	3.09%	0.495%
26	21.127	3064	3067	3073	rVB	592801	817362	4.50%	0.722%
27	21.333	3098	3102	3111	rBV3	338323	881313	4.85%	0.778%
28	21.415	3112	3116	3120	rVV	2959164	3811021	20.98%	3.366%
29	21.474	3121	3126	3131	rVB	1663658	2818262	15.51%	2.489%
30	22.274	3256	3262	3269	rVB	1242314	2592717	14.27%	2.290%
31	22.968	3373	3380	3390	rBV2	2881769	7011300	38.59%	6.193%
32	23.780	3512	3518	3528	rVB2	2082392	4061490	22.36%	3.587%
33	25.056	3727	3735	3752	rVB2	2319689	8483888	46.70%	7.494%

Sum of corrected areas: 113215716

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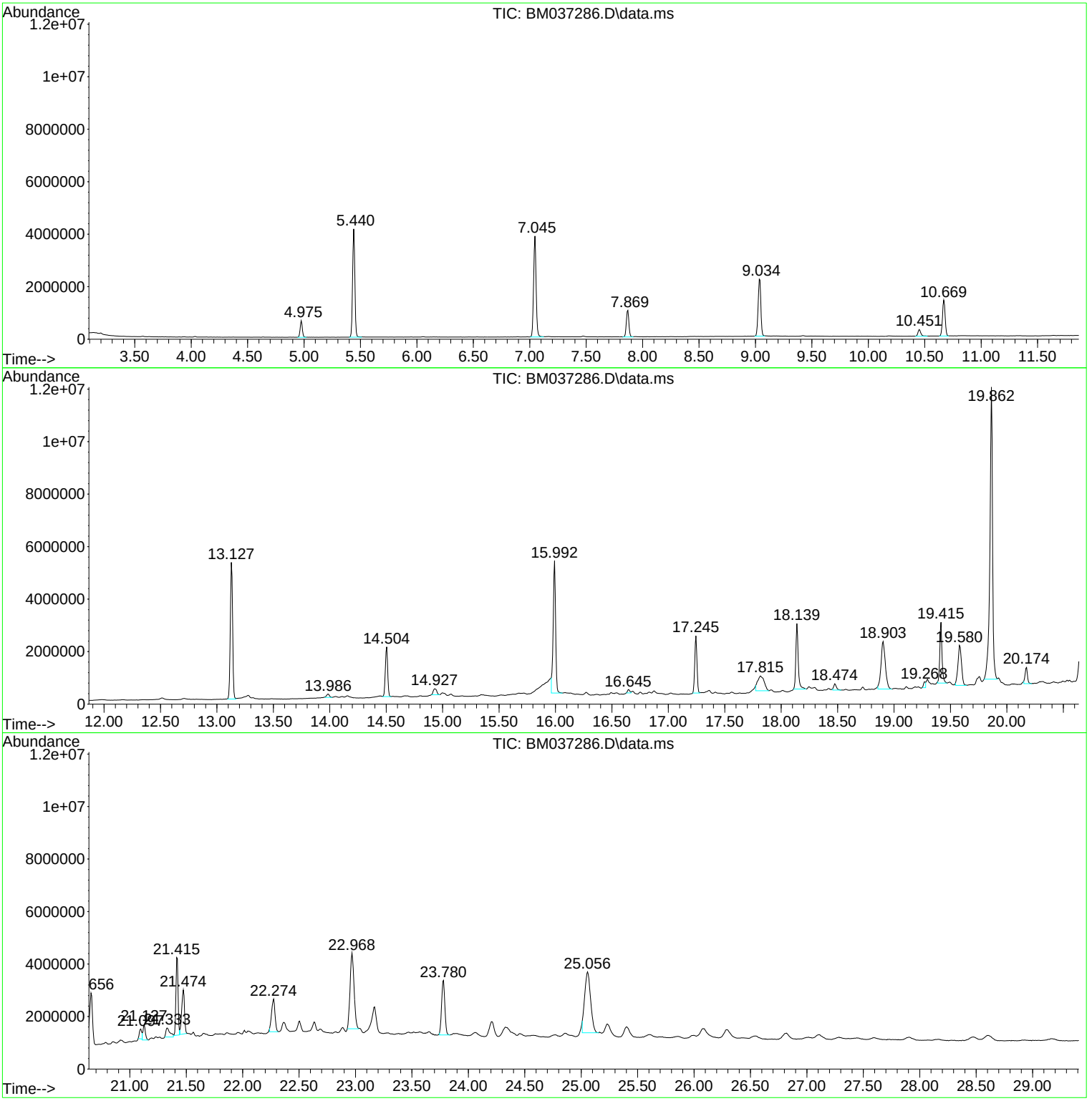
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221107-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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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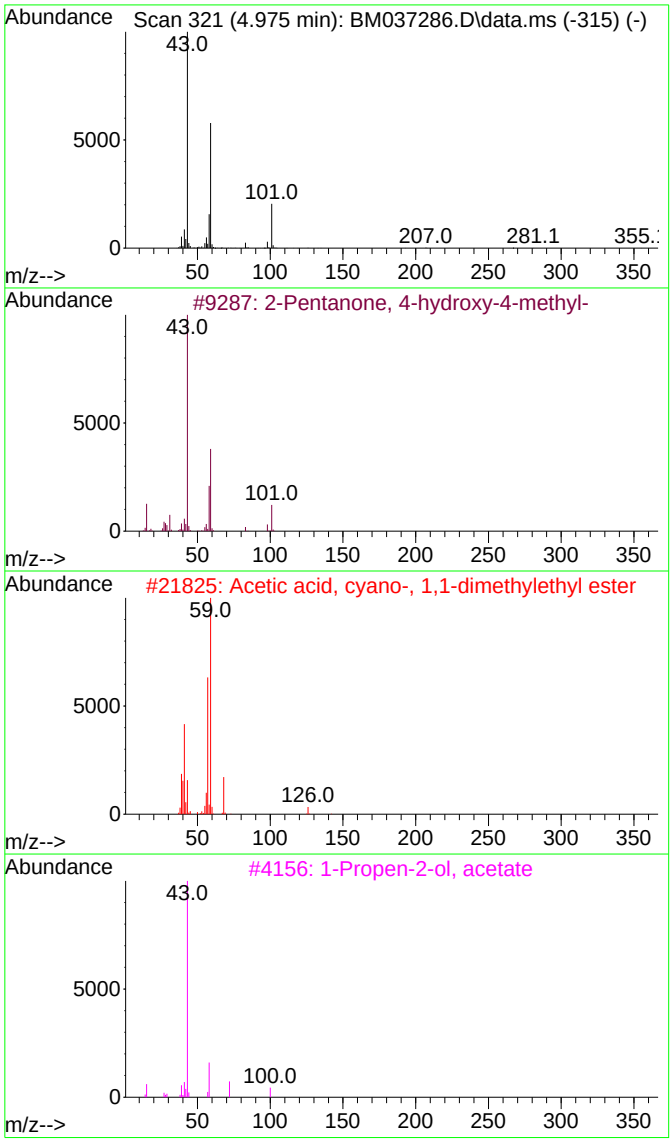
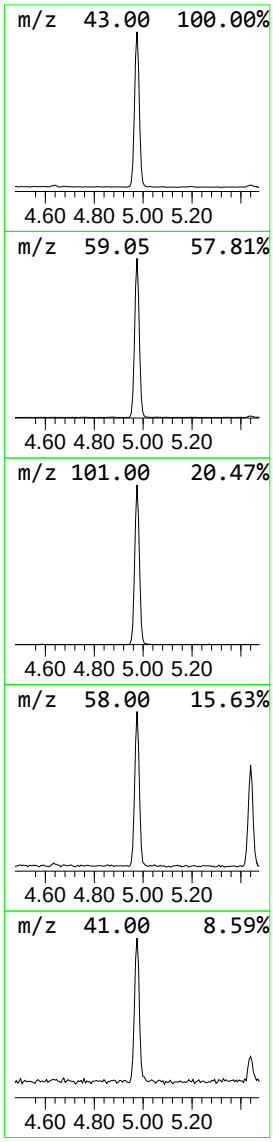
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	10.63 ng	841722	1,4-Dichlorobenzene-d4	7.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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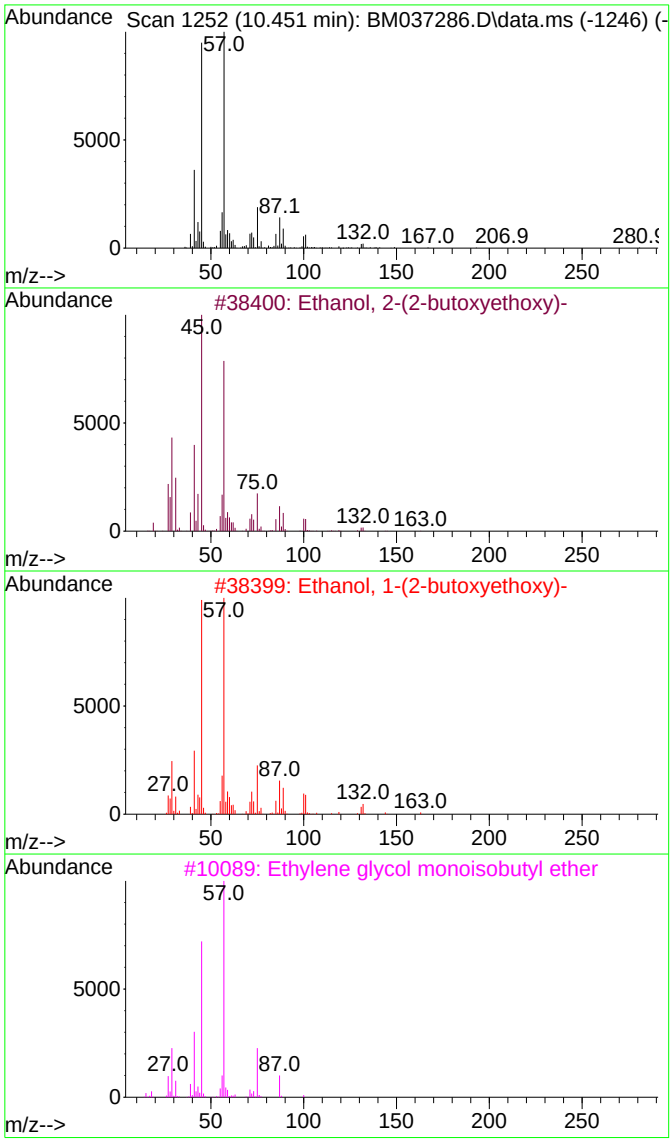
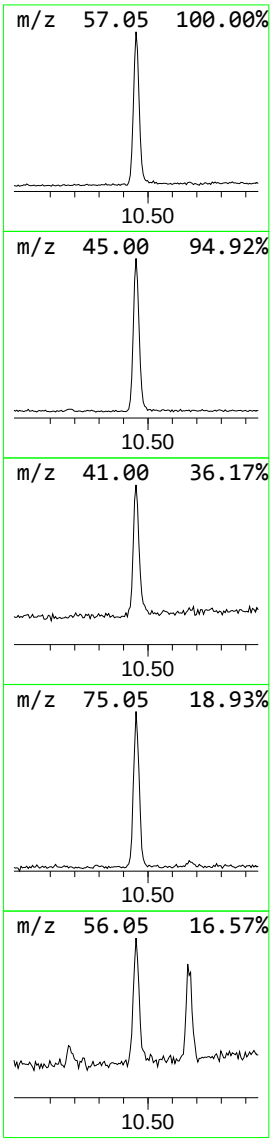
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	4.11 ng	451314	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59





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ClientSampleId :
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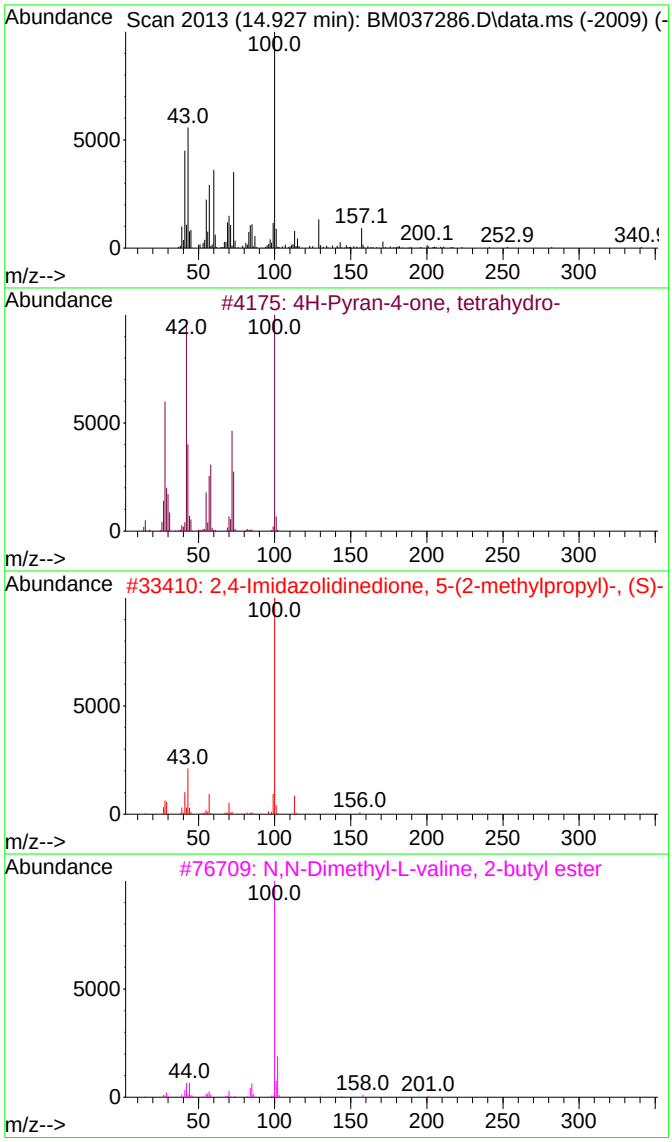
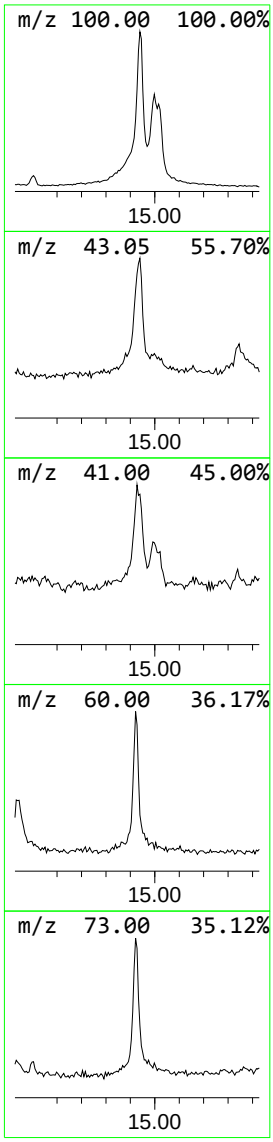
Peak Number 3 unknown14.927 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	3.56 ng	478654	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Pyran-4-one, tetrahydro-	100	C5H8O2	029943-42-8	47
2	2,4-Imidazolidinedione, 5-(2-met...	156	C7H12N2O2	040856-75-5	43
3	N,N-Dimethyl-L-valine, 2-butyl e...	201	C11H23NO2	1000451-99-4	43
4	Di-N-propylethylamine	129	C8H19N	020634-92-8	43
5	3-ACETYL-3-METHYL-.gamma.-BUTYRO...	142	C7H10O3	1000426-87-3	43





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20221107-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
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TIC Library : C:\Database\NIST20.L
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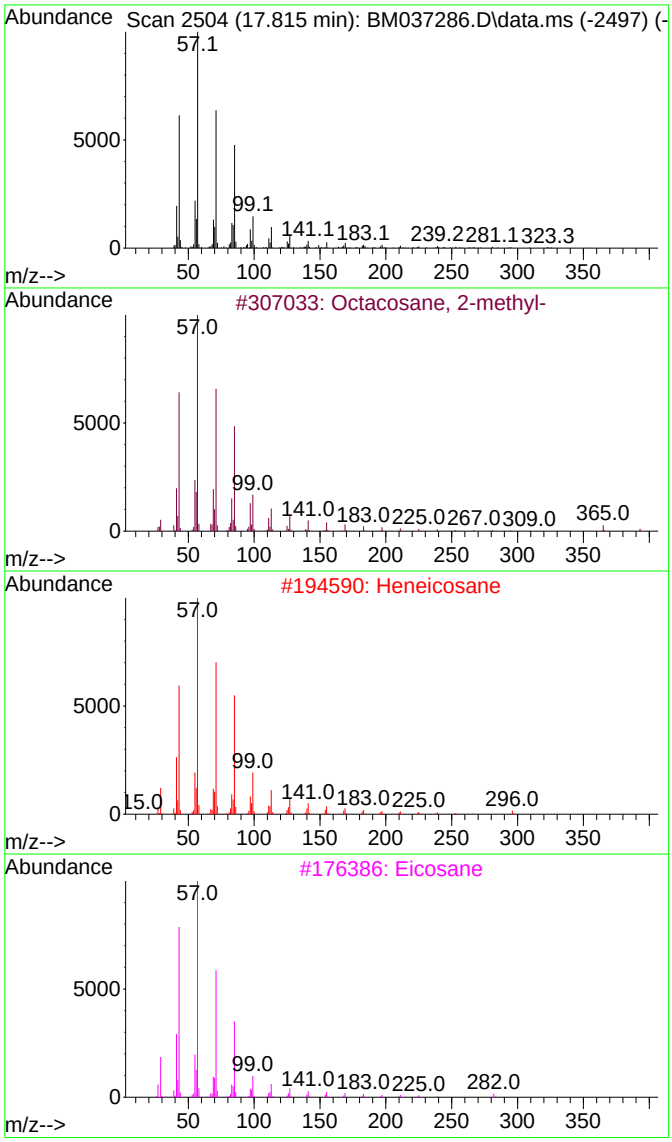
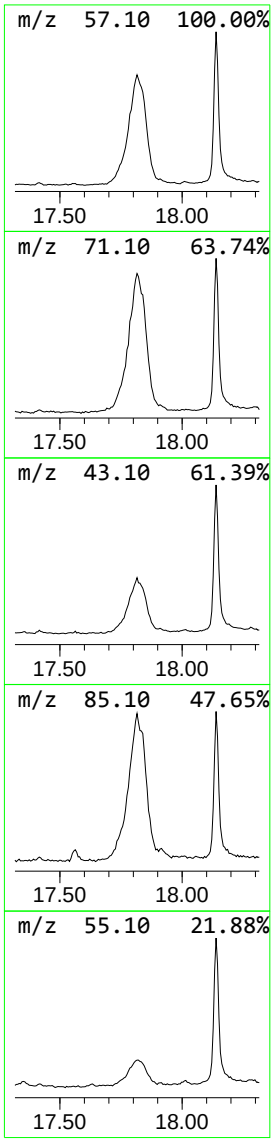
****

Peak Number 4 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.815	15.21 ng	2265220	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane	282	C20H42	000112-95-8	86
4	Nonadecane	268	C19H40	000629-92-5	83
5	Octacosane	394	C28H58	000630-02-4	83





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
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TIC Library : C:\Database\NIST20.L
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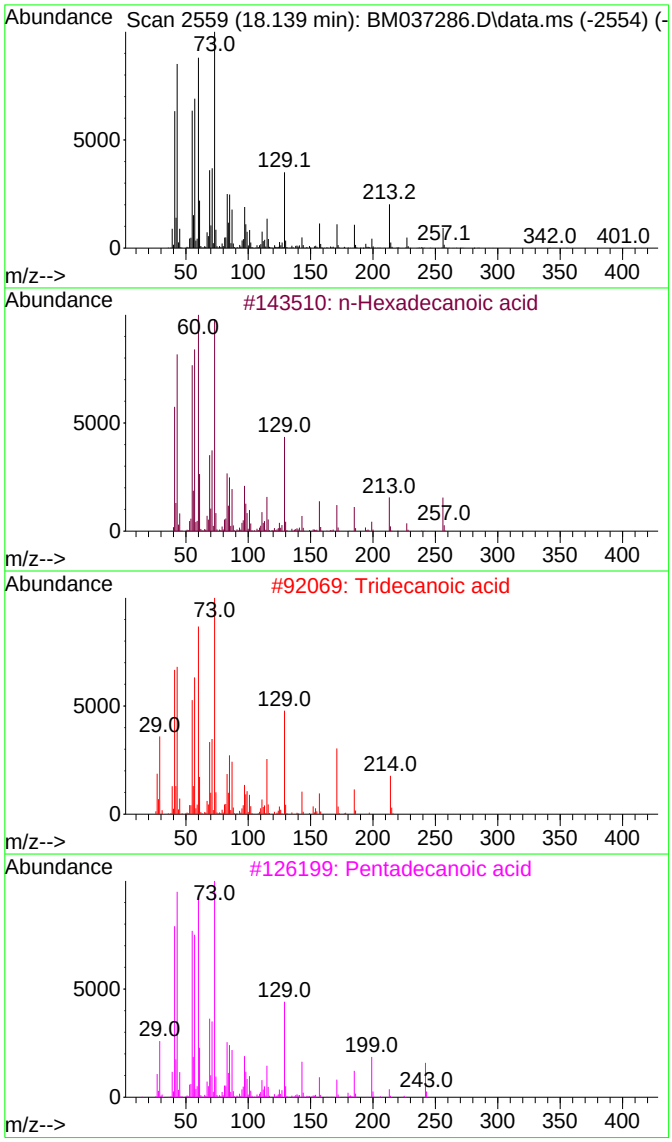
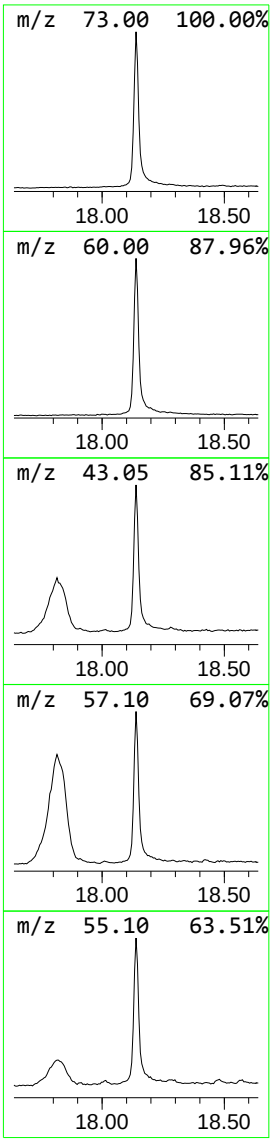
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	23.70 ng	3528310	Phenanthrene-d10	17.245

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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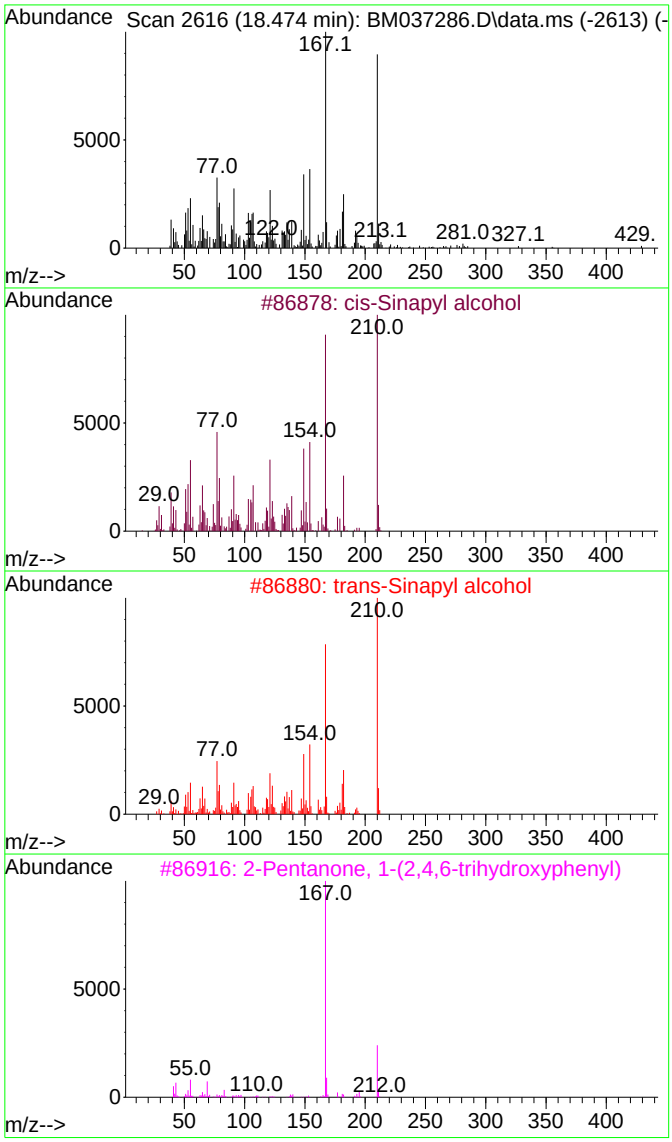
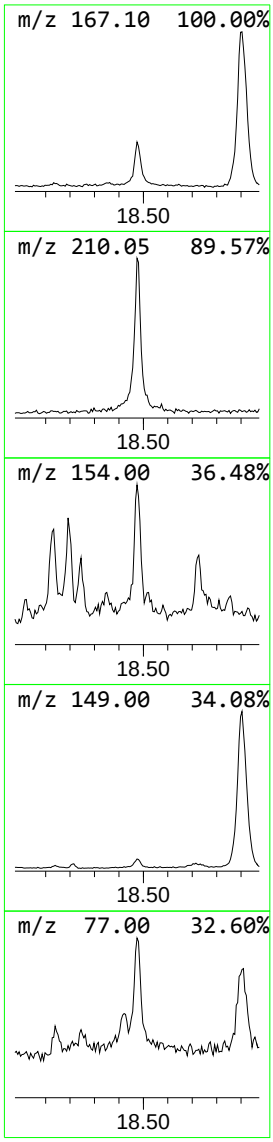
****

Peak Number 6 cis-Sinapyl alcohol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.474	2.63 ng	392070	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	94
2	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	94
3	2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	58
4	Syringylacetone	210	C11H14O4	019037-58-2	53
5	Desaspidinol	210	C11H14O4	000437-72-9	53





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Sample : N5318-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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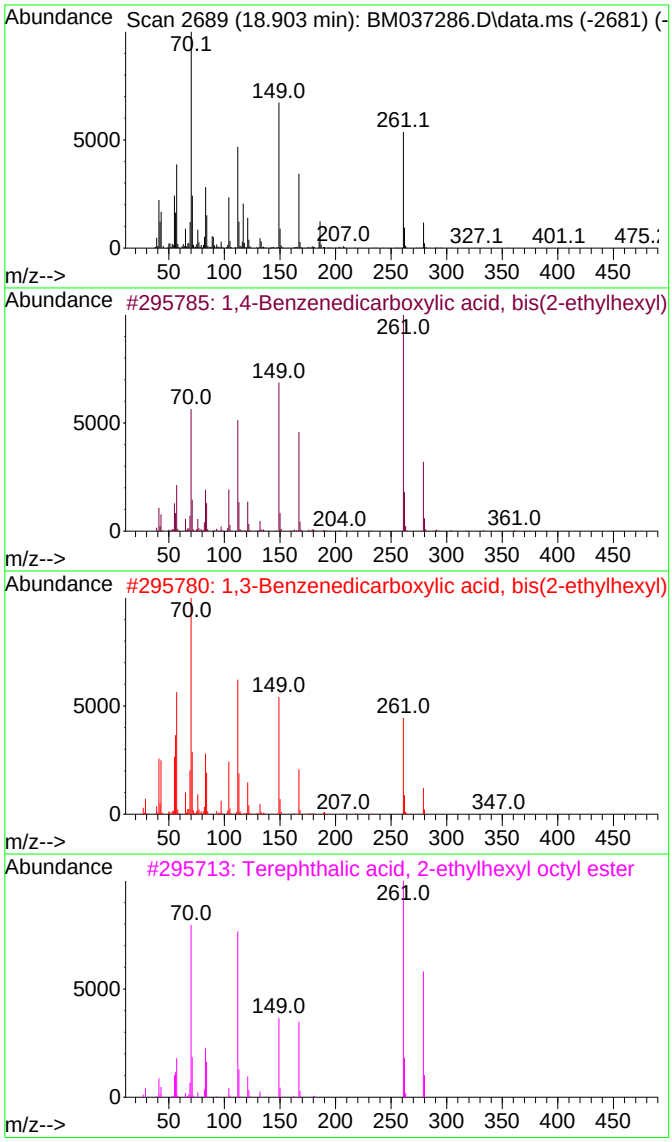
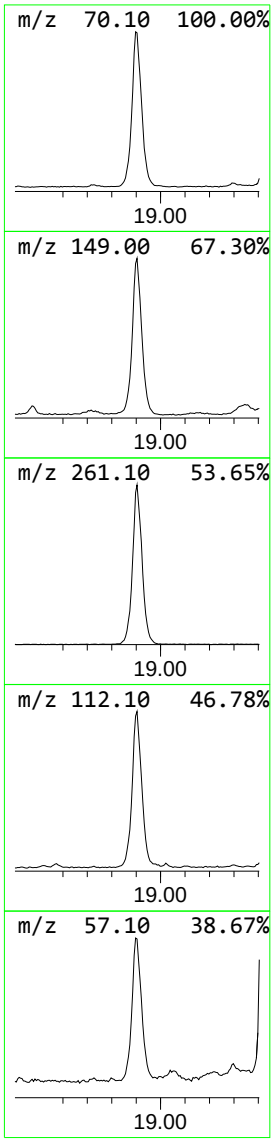
Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.904	32.23 ng	4798830	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	76
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	47
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	46
5	2-(4-Bromobenzyl)pyrrolidine, N-...	281	C13H16BrNO	1790686-43-9	30





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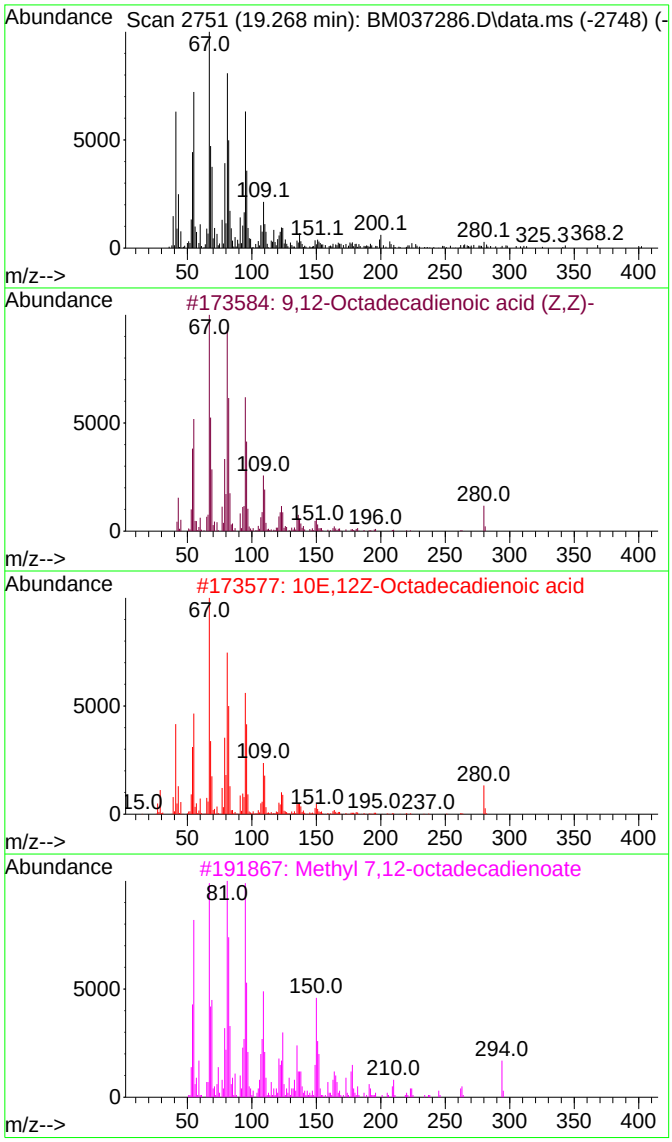
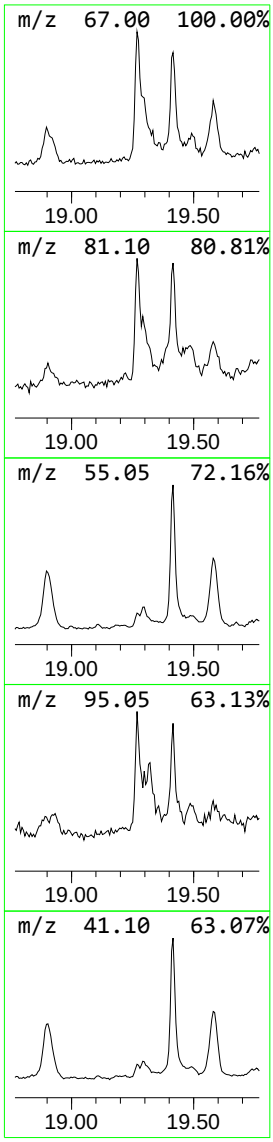
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9,12-Octadecadienoic acid (... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	2.02 ng	300044	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	94
3	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	91
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	90
5	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	83





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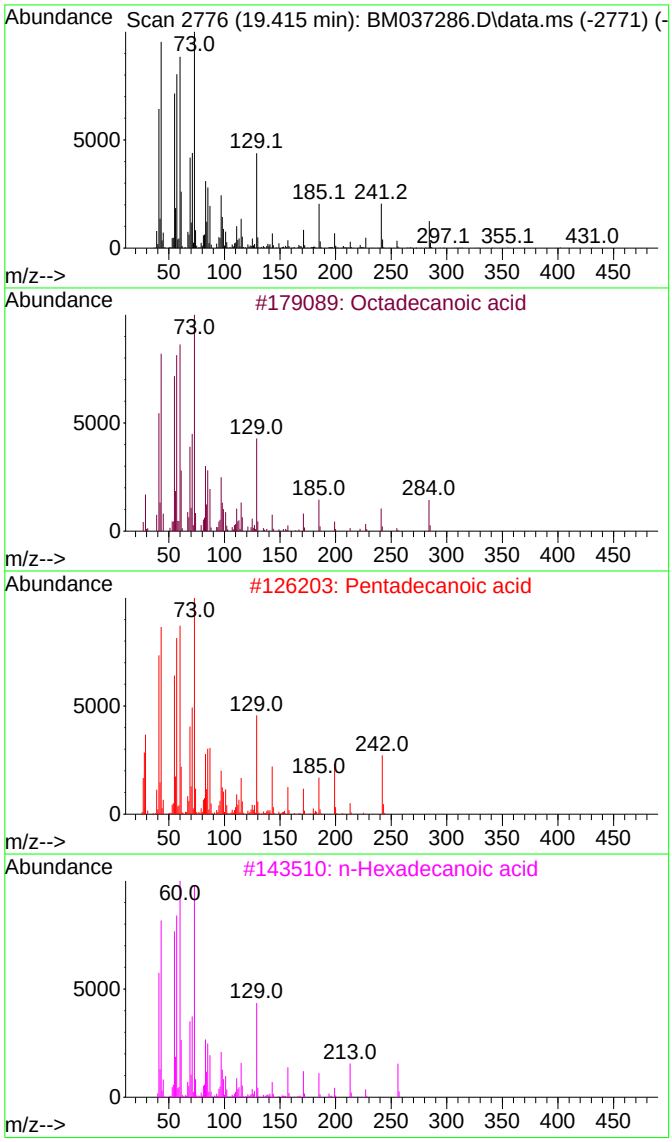
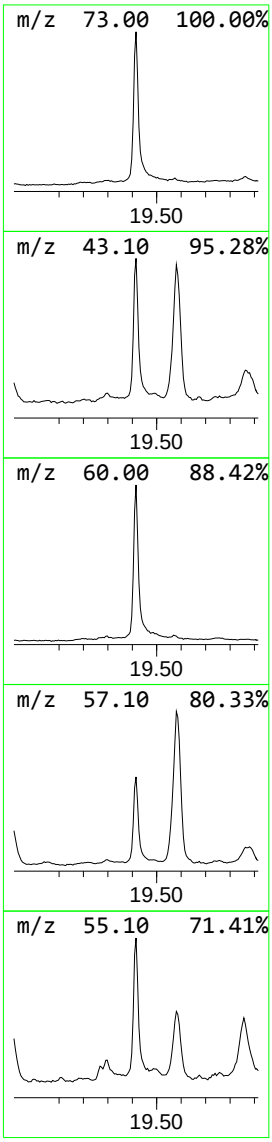
Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.415	16.52 ng	3148530	Chrysene-d12	21.415

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	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80





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Operator : CG/JU
Sample : N5318-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
20221107-COMP-06

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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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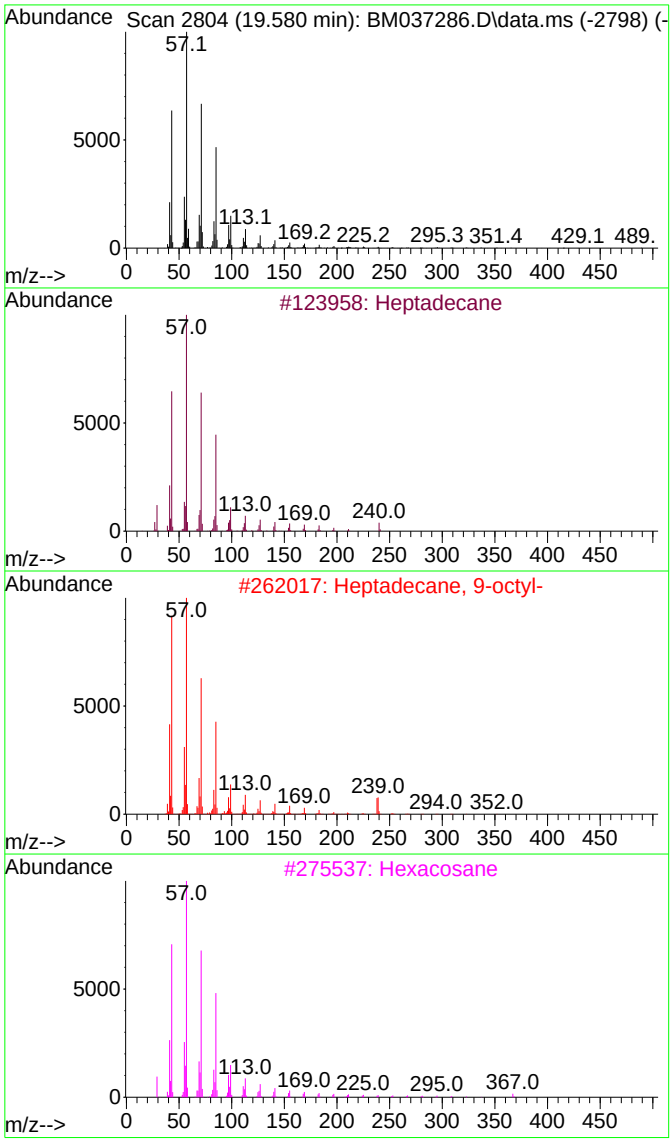
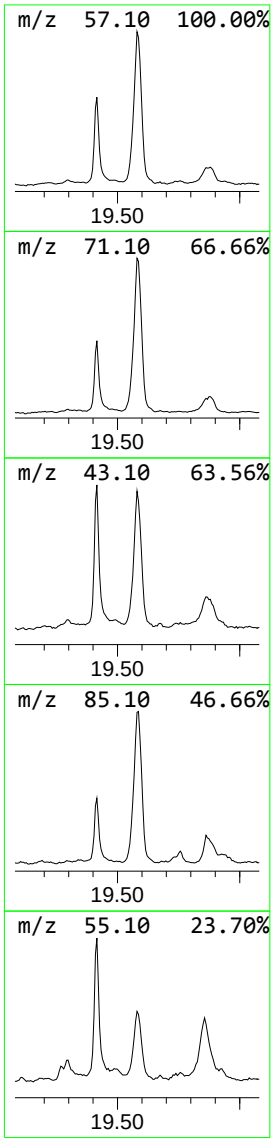
Peak Number 10 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.580	17.21 ng	3279280	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





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ClientSampleId :
20221107-COMP-06

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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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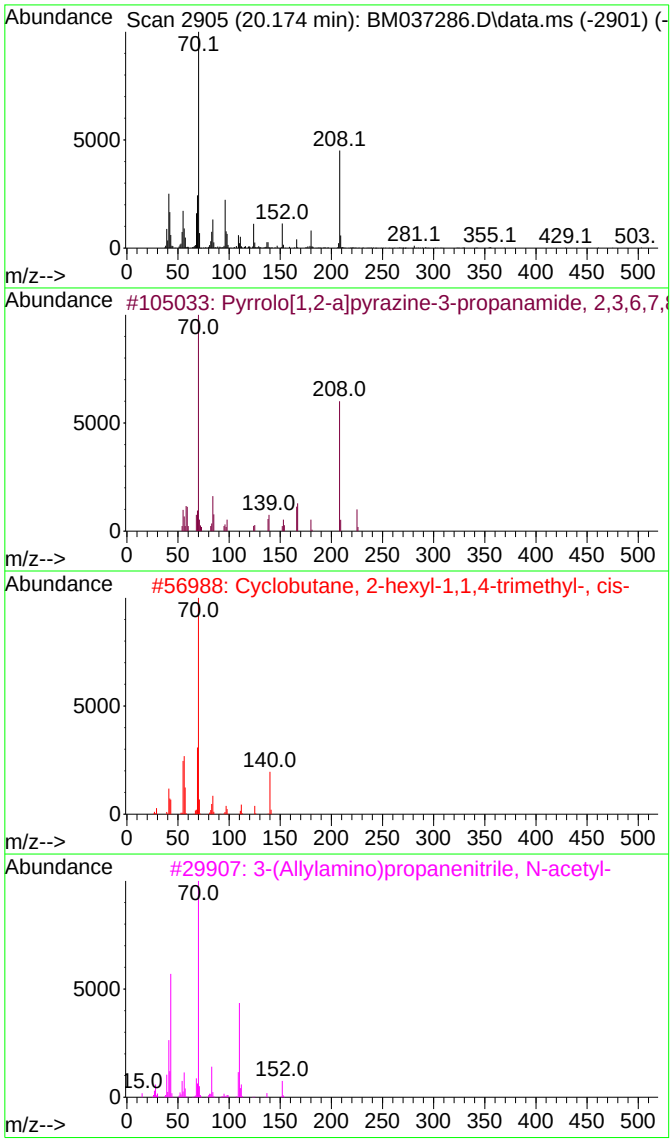
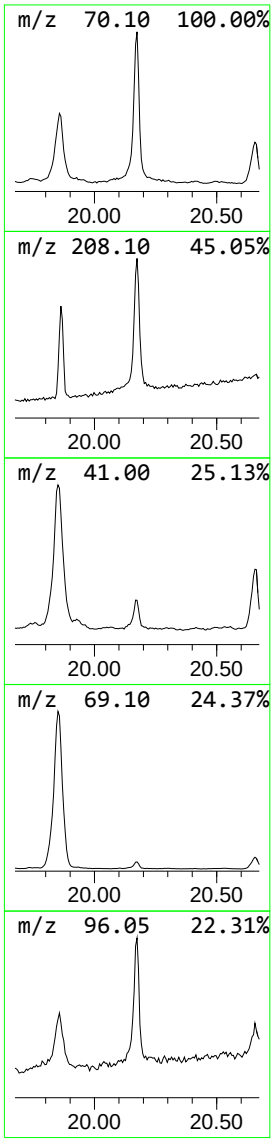
Peak Number 11 unknown20.174 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.174	4.77 ng	909220	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]pyrazine-3-propana...	225	C10H15N3O3	1000142-42-0	45
2	Cyclobutane, 2-hexyl-1,1,4-trime...	182	C13H26	049622-19-7	35
3	3-(Allylamino)propanenitrile, N-...	152	C8H12N2O	1000475-61-4	32
4	4-[p-Chlorobenzoyl]-1-methylpipe...	237	C13H16ClNO	1010250-75-8	25
5	2-Acetylpyrrolidine	113	C6H11NO	060026-20-2	25





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ClientSampleId :
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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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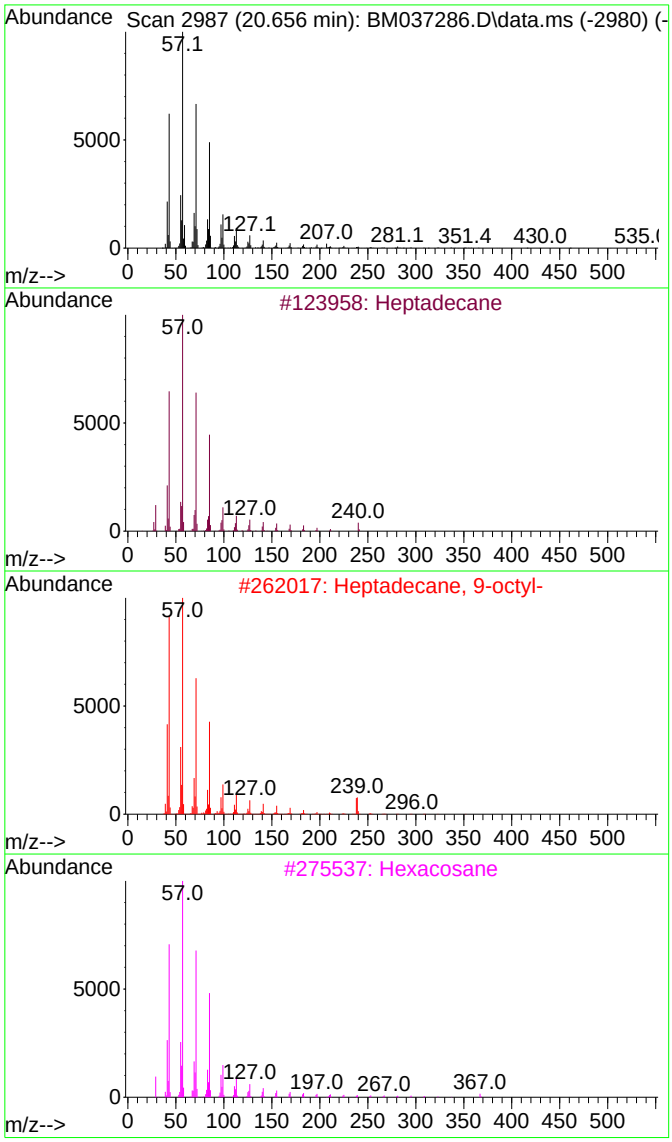
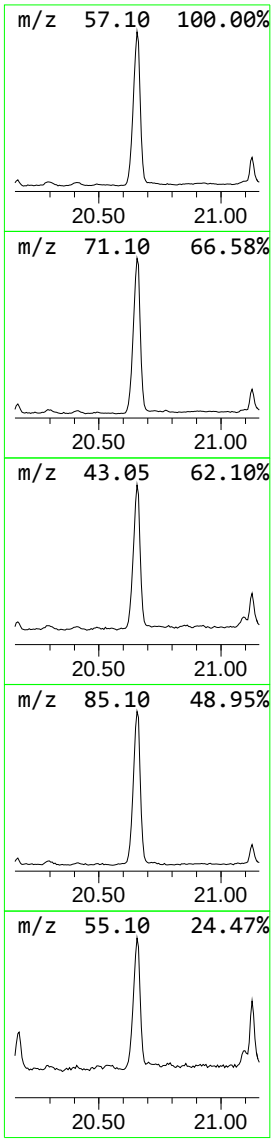
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.656	19.77 ng	3767860	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Octadecane	254	C18H38	000593-45-3	87





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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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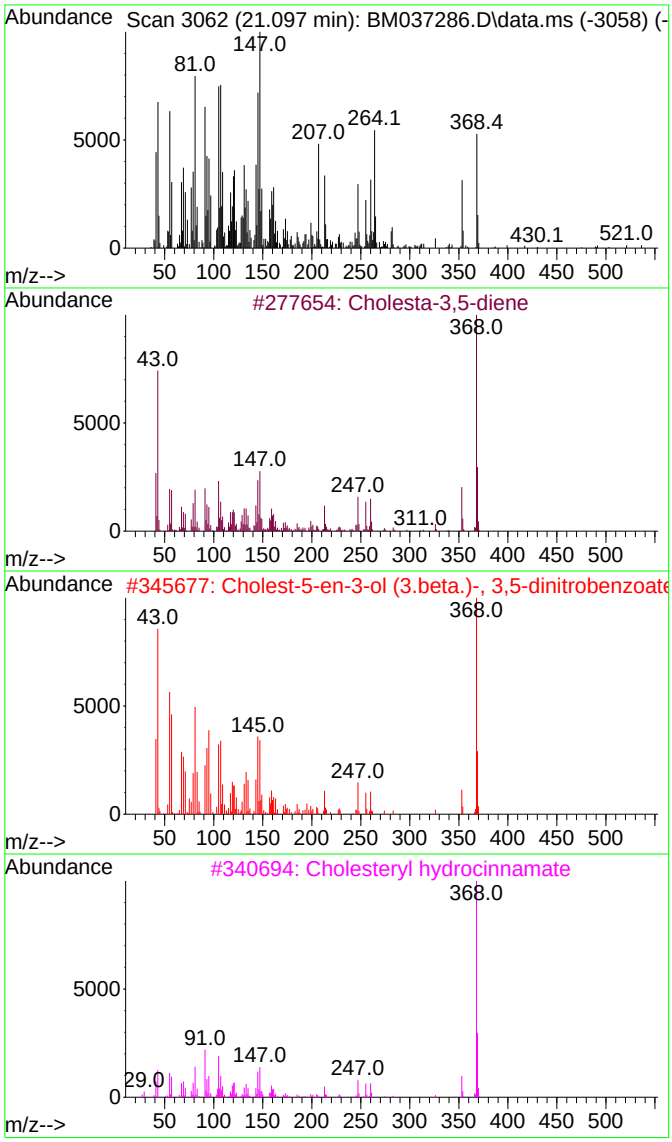
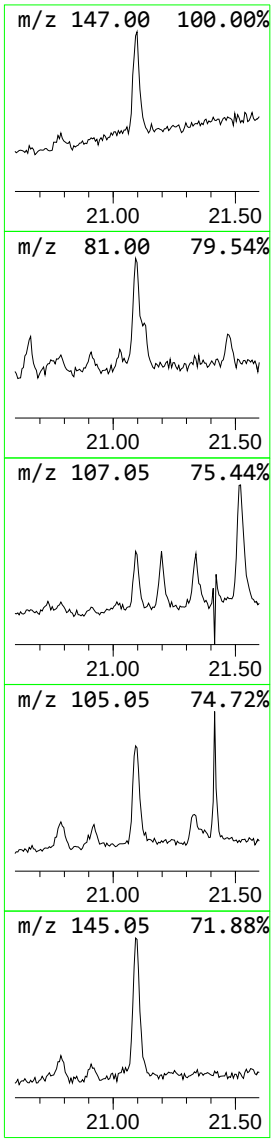
Peak Number 13 Cholesta-3,5-diene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	2.94 ng	560613	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesta-3,5-diene	368	C27H44	000747-90-0	99
2	Cholest-5-en-3-ol (3.beta.)-, 3,...	580	C34H48N2O6	025279-63-4	58
3	Cholesteryl hydrocinnamate	518	C36H54O2	014914-99-9	50
4	Cholesteryl methyl carbonate	444	C29H48O3	015507-52-5	45
5	Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	45





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ALS Vial : 5 Sample Multiplier: 1

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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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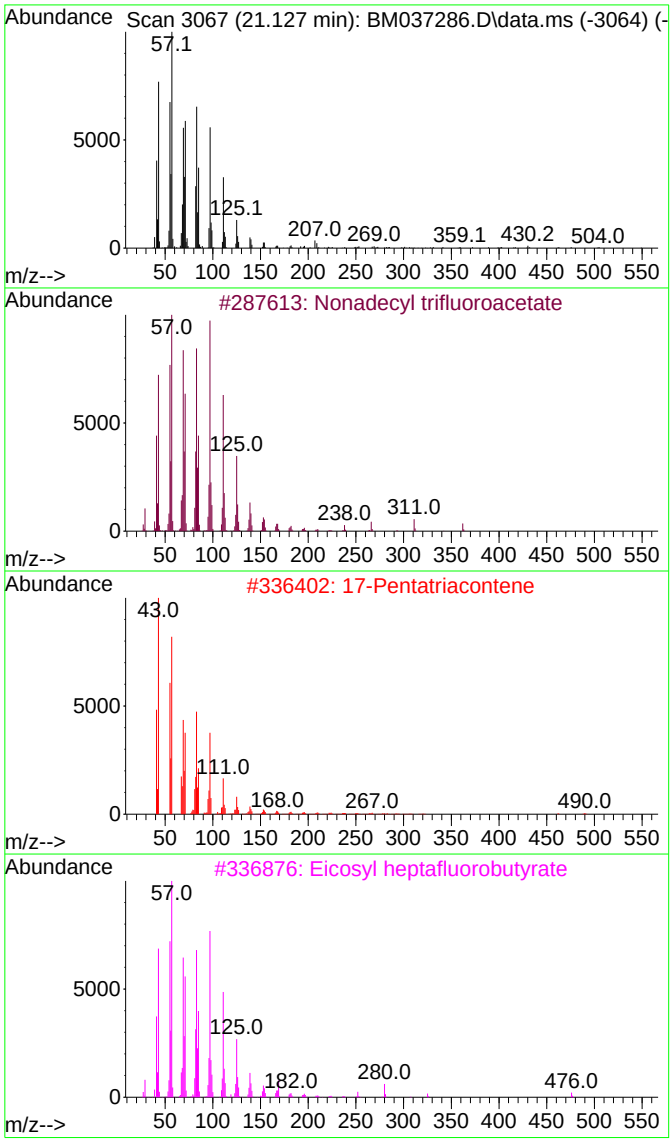
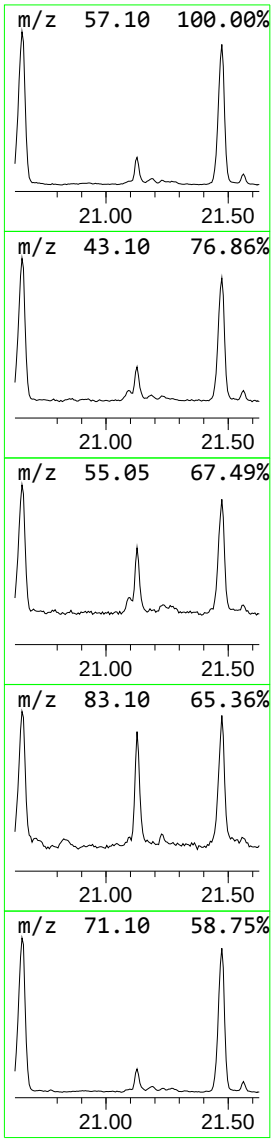
Peak Number 14 Nonadecyl trifluoroacetate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.29 ng	817362	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
4	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87





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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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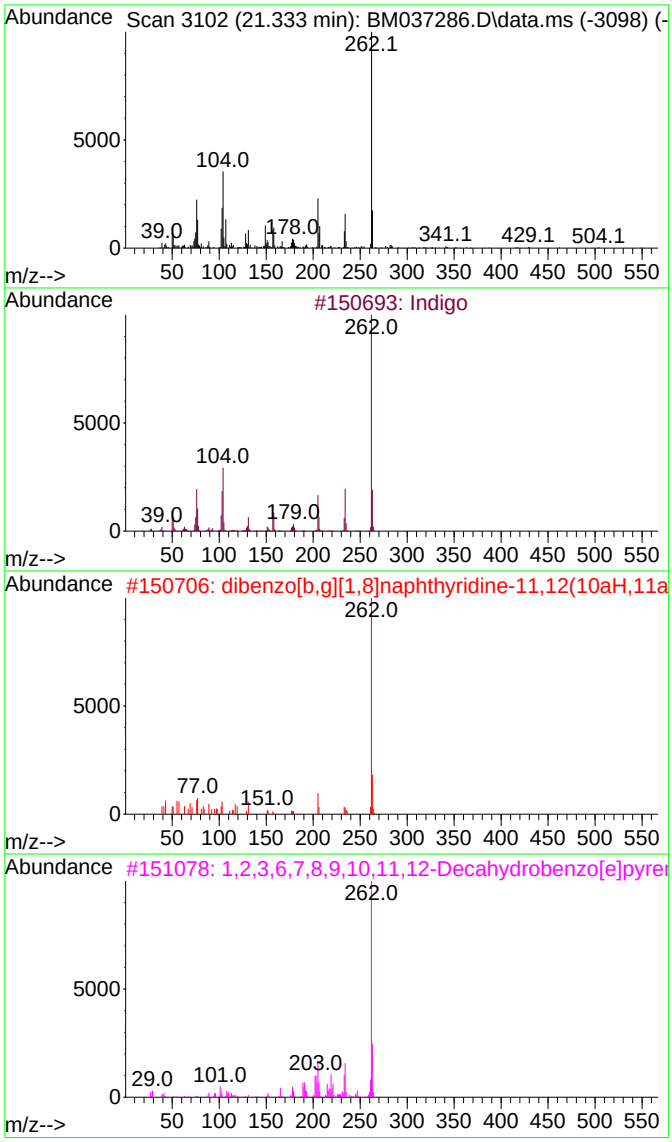
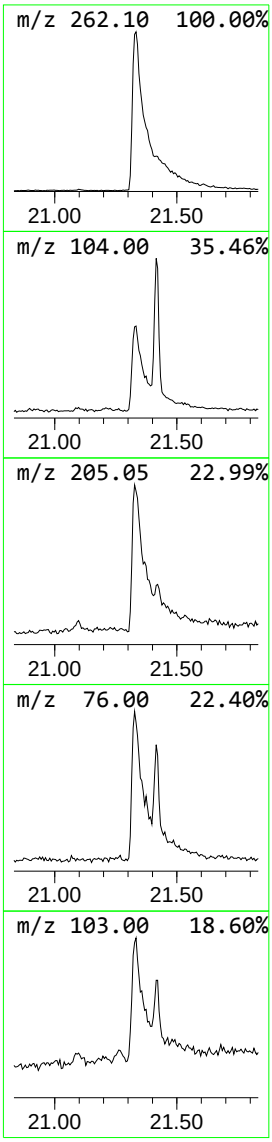
Peak Number 15 Indigo Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.333	4.63 ng	881313	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indigo	262	C16H10N2O2	000482-89-3	99
2	dibenzo[b,g][1,8]naphthyridine-1...	262	C16H10N2O2	1000396-82-0	53
3	1,2,3,6,7,8,9,10,11,12-Decahydro...	262	C20H22	092387-50-3	50
4	1,1'-Binaphthalene, 5,5',6,6',7,...	262	C20H22	001154-14-9	50
5	2,4,6(1H,3H,5H)-Pyrimidinetrione...	262	C12H14N4O3	1000350-66-3	49





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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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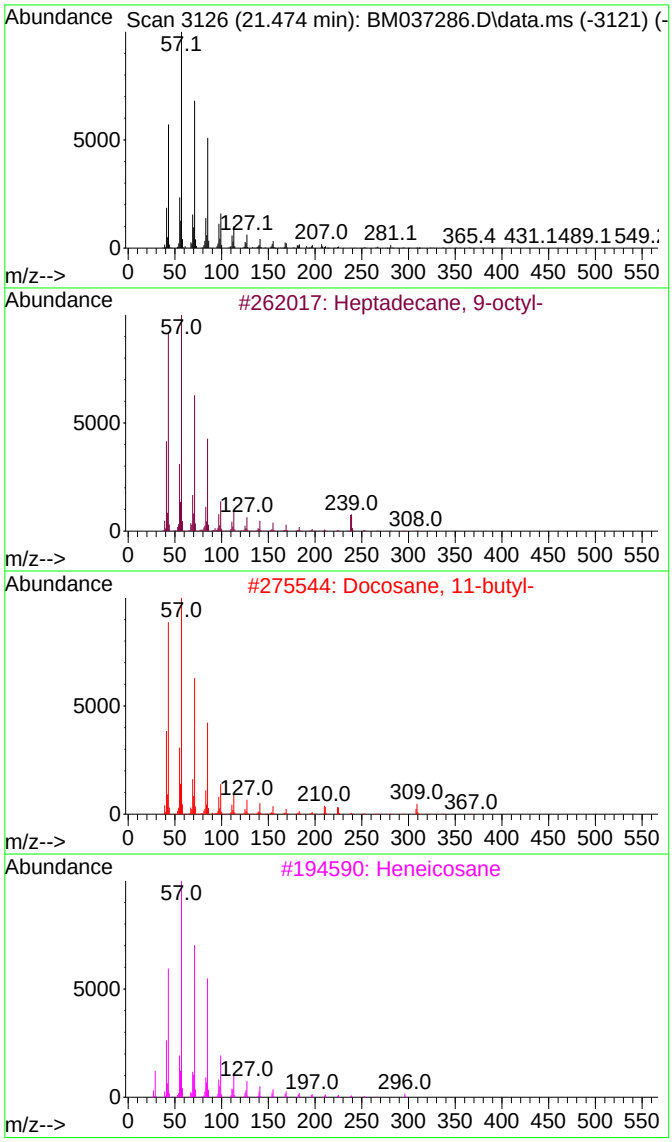
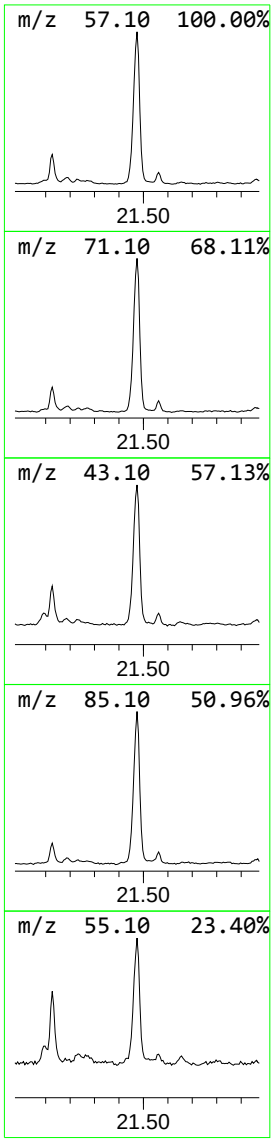
Peak Number 16 Docosane, 11-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	14.79 ng	2818260	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





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ClientSampleId :
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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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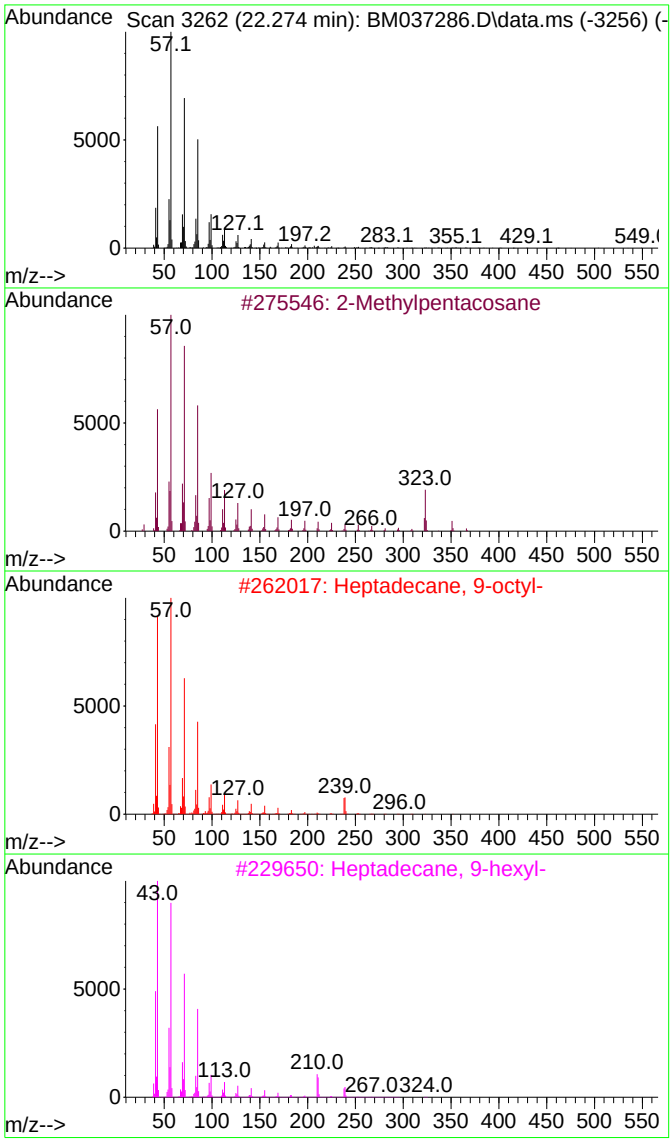
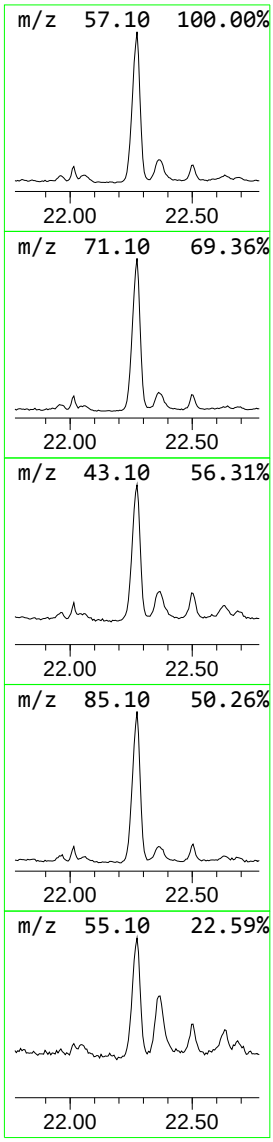
Peak Number 17 2-Methylpentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.274	13.61 ng	2592720	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylpentacosane	366	C26H54	000629-87-8	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
5	Tricosane	324	C23H48	000638-67-5	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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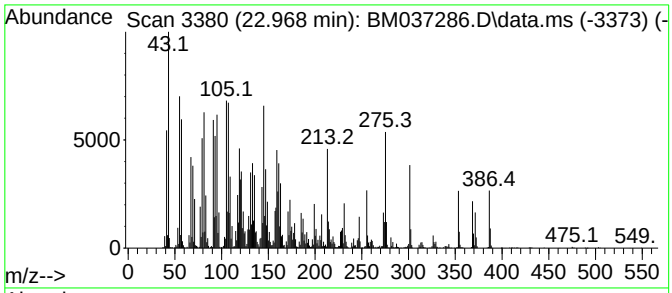
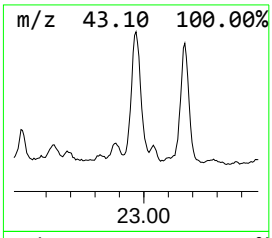
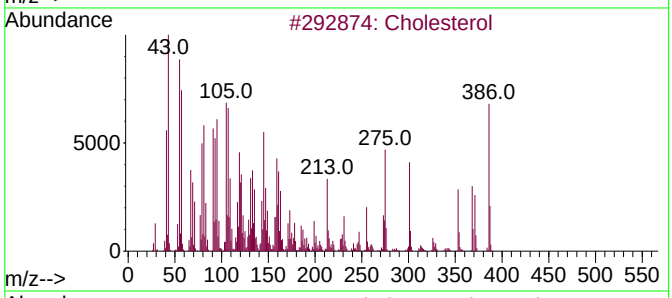
Peak Number 18 Cholesterol Concentration Rank 2

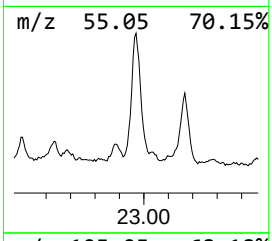
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.968	34.53 ng	7011300	Perylene-d12	23.780

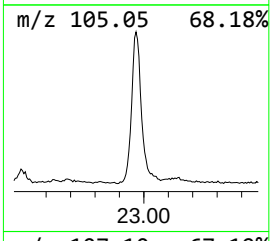
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	Lathosterol	386	C27H46O	000080-99-9	84
4	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	53
5	Boscartol F	300	C20H28O2	1486443-17-7	45

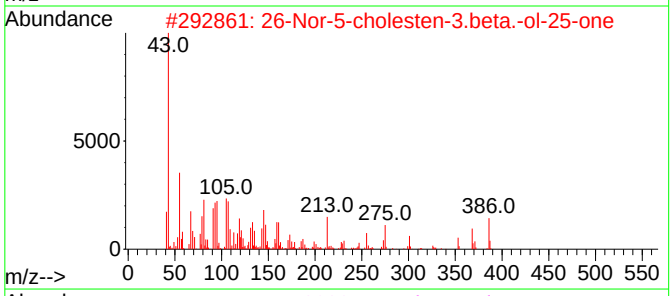


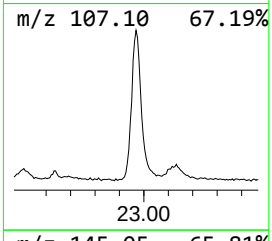


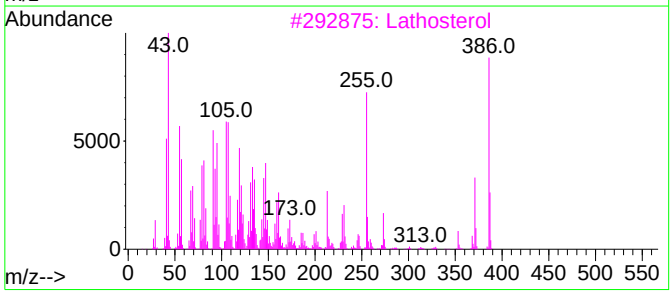


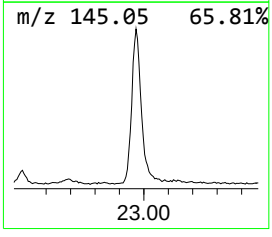












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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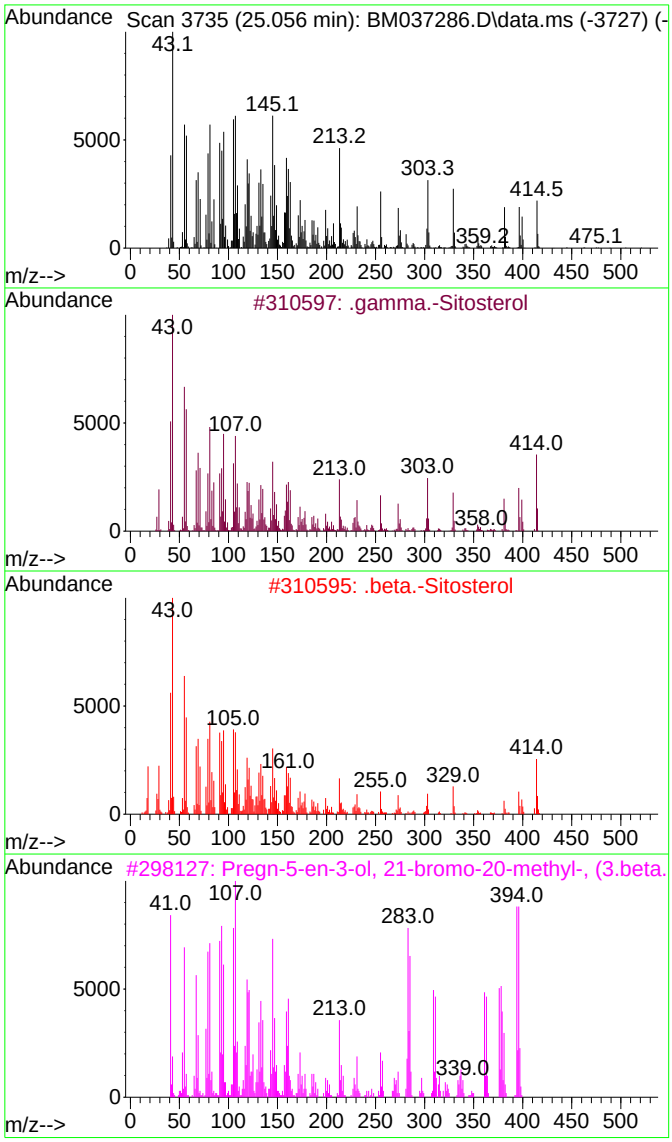
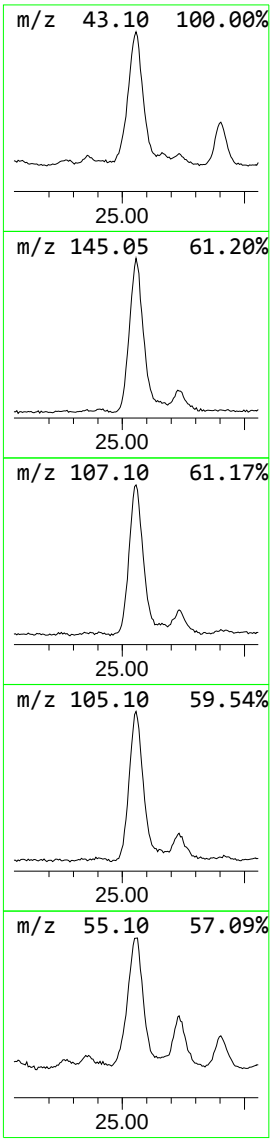
Peak Number 19 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.056	41.78 ng	8483890	Perylene-d12	23.780

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	93
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	91
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	89
5	Campesterol	400	C28H48O	000474-62-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
Data File : BM037286.D
Acq On : 31 Oct 2022 12:40
Operator : CG/JU
Sample : N5318-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20221107-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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-...	4.975	10.6	ng	841722	1	7.869	1582970	20.0
Ethanol, 2-(2-b...	10.451	4.1	ng	451314	2	10.669	2194210	20.0
unknown14.927	14.927	3.6	ng	478654	3	14.504	2692290	20.0
Octacosane, 2-m...	17.815	15.2	ng	2265220	4	17.245	2977750	20.0
n-Hexadecanoic ...	18.139	23.7	ng	3528310	4	17.245	2977750	20.0
cis-Sinapyl alc...	18.474	2.6	ng	392070	4	17.245	2977750	20.0
1,4-Benzenedica...	18.904	32.2	ng	4798830	4	17.245	2977750	20.0
9,12-Octadecadi...	19.268	2.0	ng	300044	4	17.245	2977750	20.0
Octadecanoic acid	19.415	16.5	ng	3148530	5	21.415	3811020	20.0
Heptadecane	19.580	17.2	ng	3279280	5	21.415	3811020	20.0
unknown20.174	20.174	4.8	ng	909220	5	21.415	3811020	20.0
Heptadecane, 9-...	20.656	19.8	ng	3767860	5	21.415	3811020	20.0
Cholesta-3,5-diene	21.098	2.9	ng	560613	5	21.415	3811020	20.0
Nonadecyl trifl...	21.127	4.3	ng	817362	5	21.415	3811020	20.0
Indigo	21.333	4.6	ng	881313	5	21.415	3811020	20.0
Docosane, 11-bu...	21.474	14.8	ng	2818260	5	21.415	3811020	20.0
2-Methylpentaco...	22.274	13.6	ng	2592720	5	21.415	3811020	20.0
Cholesterol	22.968	34.5	ng	7011300	6	23.780	4061490	20.0
.gamma.-Sitosterol	25.056	41.8	ng	8483890	6	23.780	4061490	20.0