

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050619\
 Data File : BM020137.D
 Acq On : 06 May 2019 16:00
 Operator : JU/SJ
 Sample : K2647-03 5X
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SU-04-050219-B

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BM043019.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	399	405	414	rBV	457096	661056	6.26%	1.569%
2	6.952	666	674	682	rBV	474520	733288	6.94%	1.741%
3	7.322	731	737	744	rBV	479993	747126	7.07%	1.774%
4	7.793	811	817	823	rBV	573296	894205	8.47%	2.123%
5	8.110	864	871	877	rVB	350048	559599	5.30%	1.329%
6	8.957	1007	1015	1025	rBV	250837	455013	4.31%	1.080%
7	10.587	1285	1292	1300	rVB	730494	1215307	11.51%	2.885%
8	13.051	1705	1711	1717	rBV	666169	979704	9.28%	2.326%
9	13.240	1739	1743	1750	rVB	86056	124556	1.18%	0.296%
10	13.892	1848	1854	1858	rVB2	109140	165868	1.57%	0.394%
11	14.316	1921	1926	1931	rBV	116868	148969	1.41%	0.354%
12	14.434	1940	1946	1953	rVB2	1055412	1624798	15.38%	3.858%
13	15.269	2083	2088	2093	rBV	122131	160609	1.52%	0.381%
14	15.922	2194	2199	2207	rVB	520772	769834	7.29%	1.828%
15	16.133	2230	2235	2244	rBV	131100	240335	2.28%	0.571%
16	16.922	2365	2369	2373	rBV	122823	154639	1.46%	0.367%
17	17.180	2407	2413	2419	rBV2	1390858	2042155	19.34%	4.849%
18	17.663	2491	2495	2500	rBV	101802	145424	1.38%	0.345%
19	17.839	2520	2525	2531	rVB	2062435	2577484	24.41%	6.119%
20	18.063	2559	2563	2567	rBV3	155066	219674	2.08%	0.522%
21	18.357	2609	2613	2617	rVB2	101258	131959	1.25%	0.313%
22	18.992	2715	2721	2723	rBV	6445414	8014154	75.88%	19.027%
23	19.022	2723	2726	2737	rVB	8519210	10561086	100.00%	25.074%
24	19.151	2744	2748	2753	rBV	900032	998122	9.45%	2.370%
25	19.204	2754	2757	2759	rBV	178336	228549	2.16%	0.543%
26	19.233	2759	2762	2768	rVB2	405385	676105	6.40%	1.605%
27	19.522	2808	2811	2816	rVB2	280095	348043	3.30%	0.826%
28	19.610	2822	2826	2833	rVB	218471	308393	2.92%	0.732%
29	19.810	2856	2860	2864	rBV	1061367	1200326	11.37%	2.850%
30	20.016	2893	2895	2898	rBV4	173102	186725	1.77%	0.443%
31	21.368	3121	3125	3130	rBV	1927639	2500681	23.68%	5.937%
32	23.662	3511	3515	3524	rVB2	1242054	2345479	22.21%	5.569%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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-BM043019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

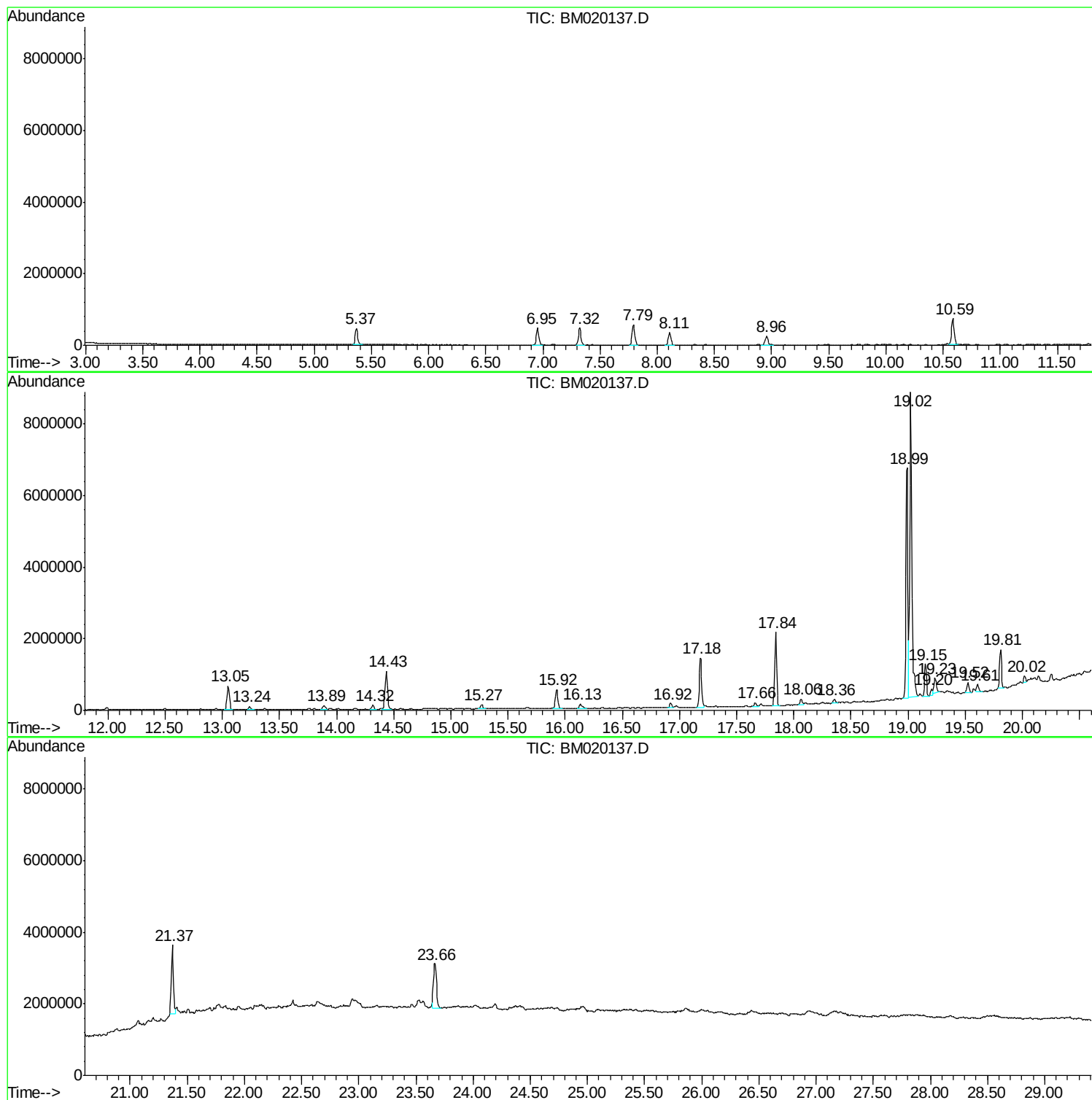
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampled :
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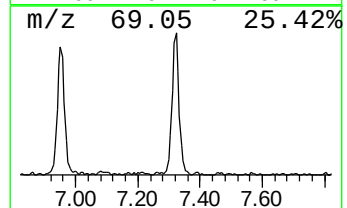
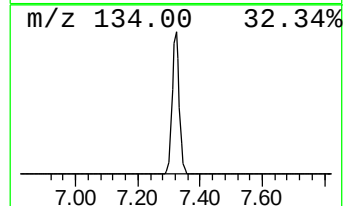
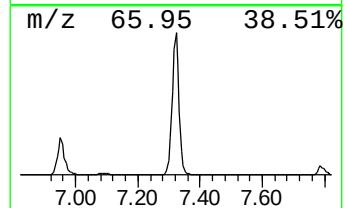
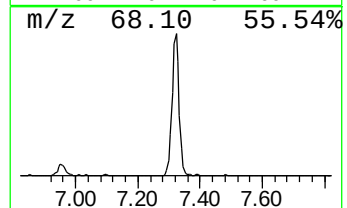
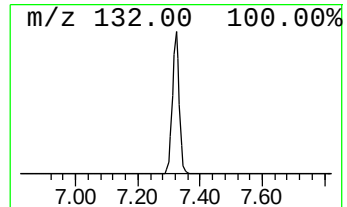
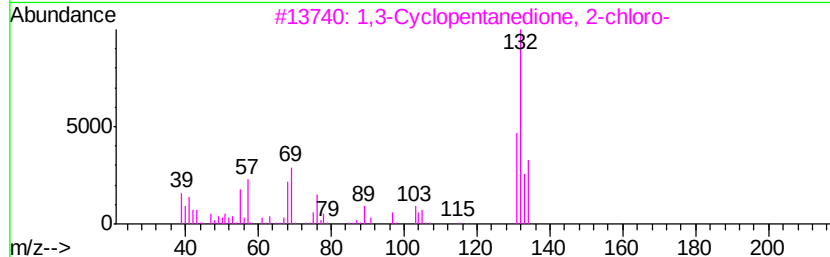
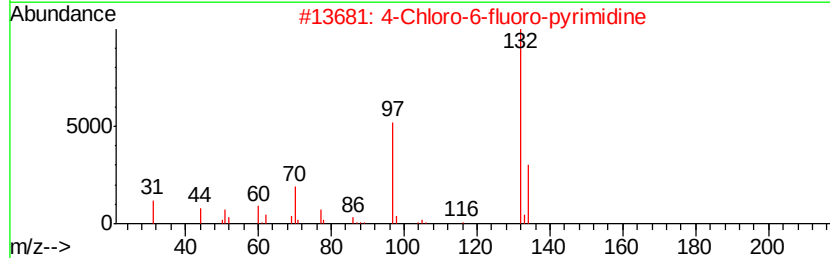
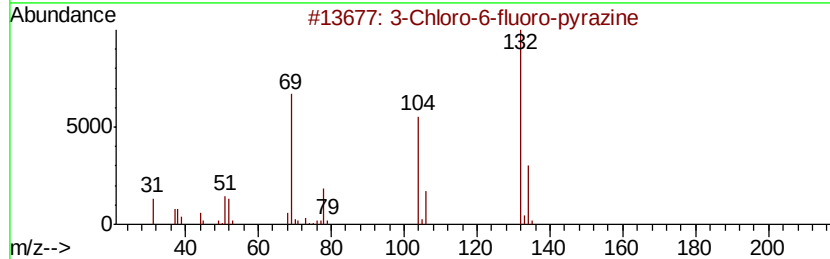
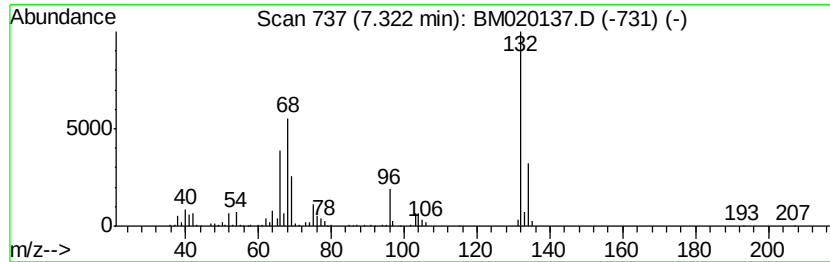
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.32 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	16.71 ng	747126	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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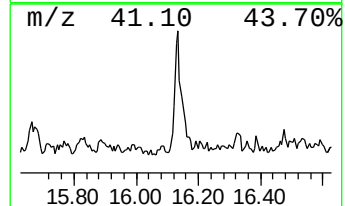
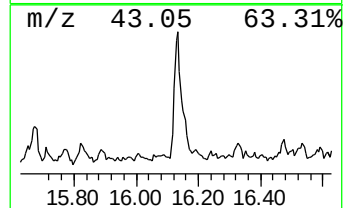
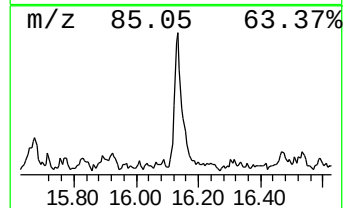
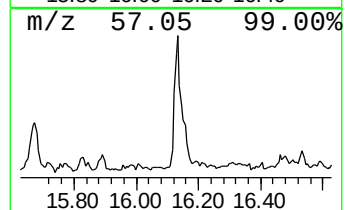
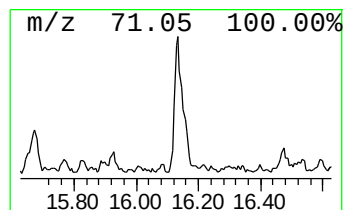
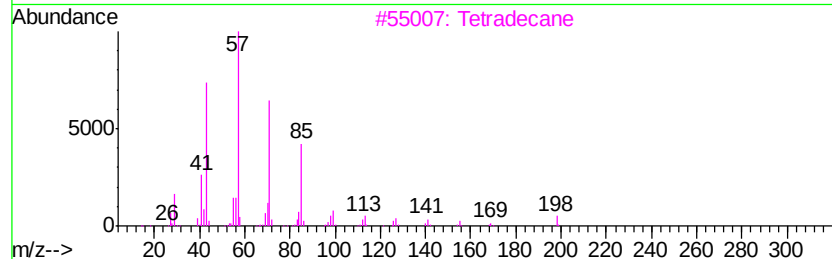
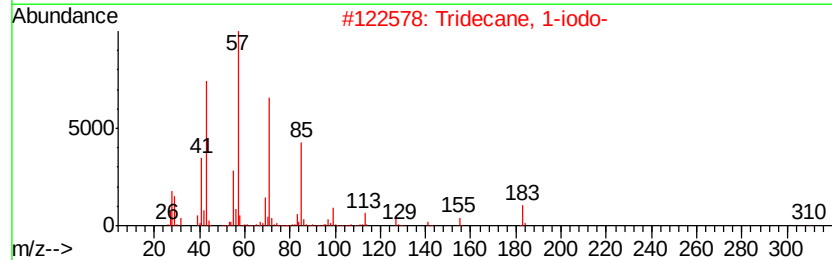
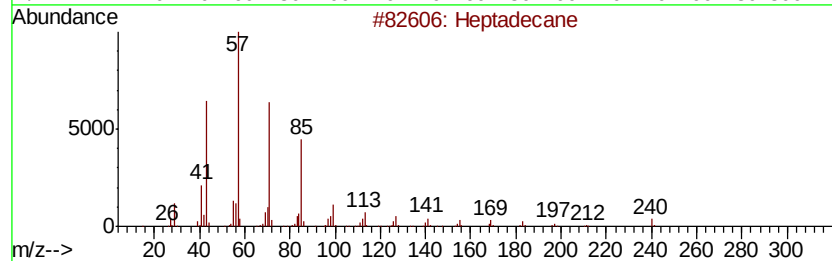
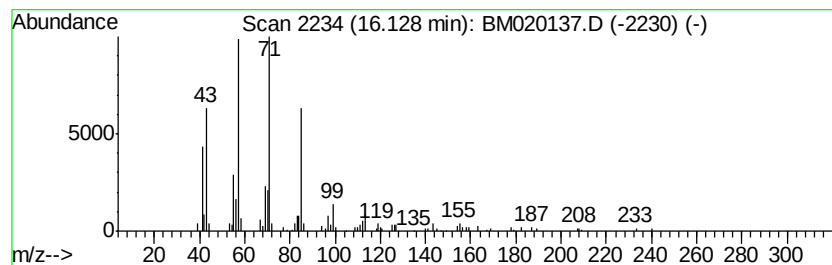
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.13	2.35 ng	240335	Phenanthrene-d10		17.18
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Tritetracontane	605	C43H88	007098-21-7	80
5	Hexadecane	226	C16H34	000544-76-3	80



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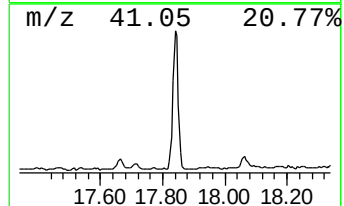
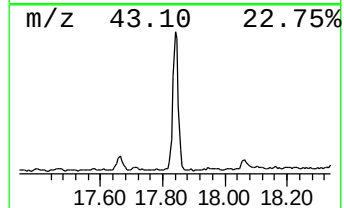
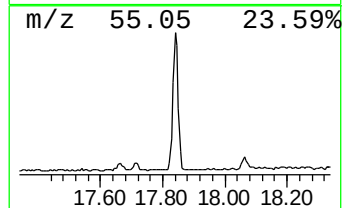
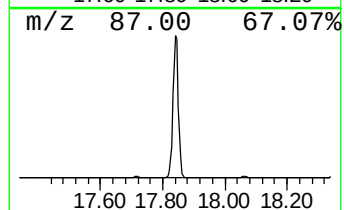
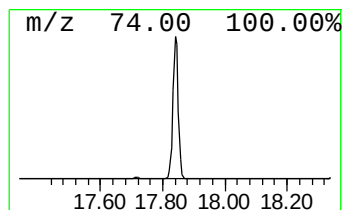
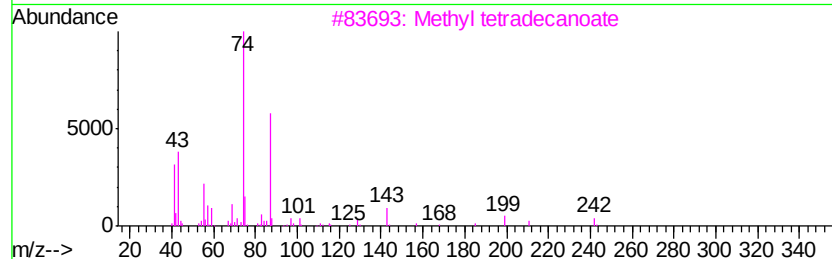
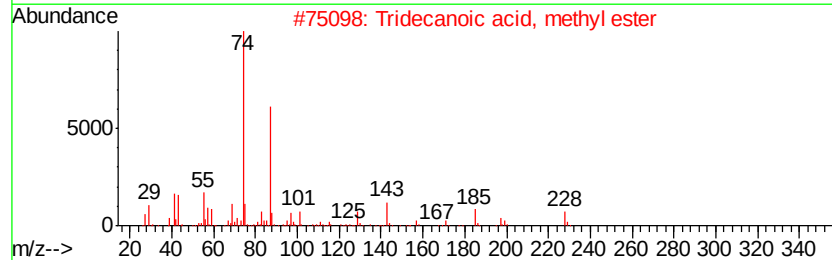
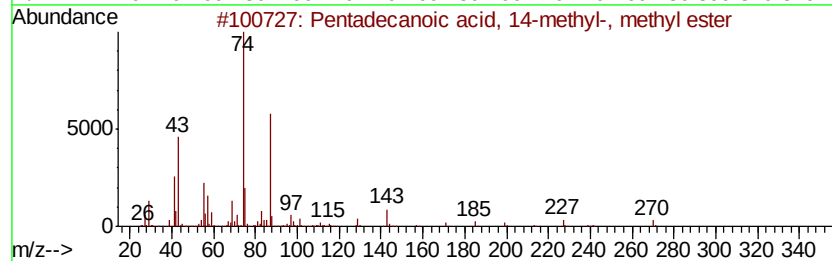
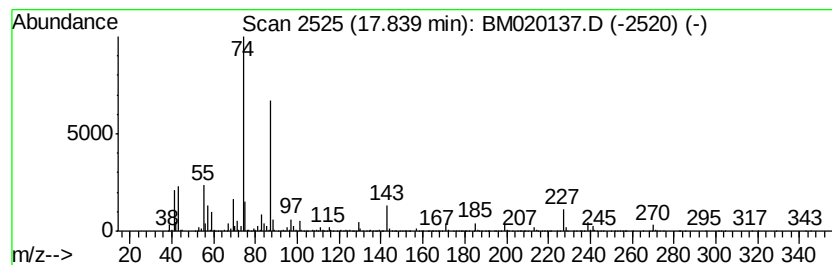
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecanoic acid, 14-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.84	25.24 ng	2577480	Phenanthrene-d10	17.18		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
2		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
5		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	90



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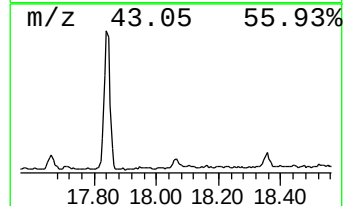
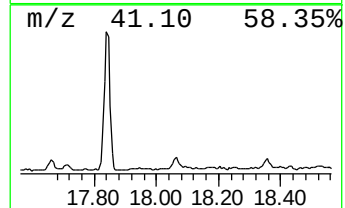
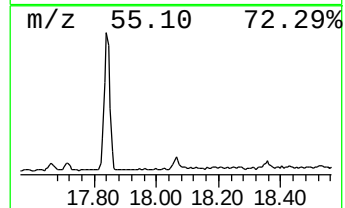
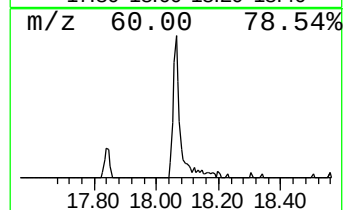
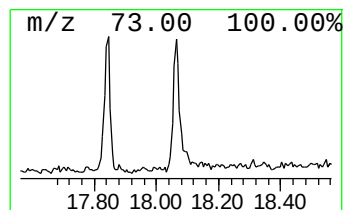
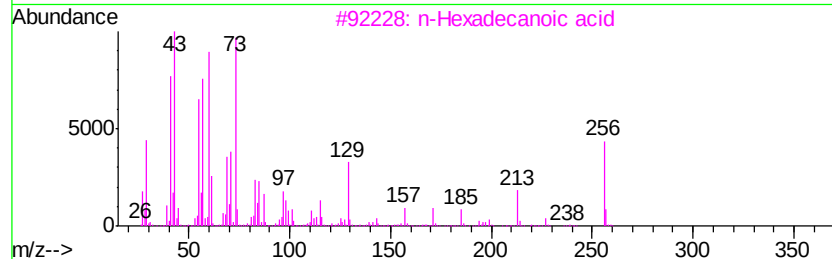
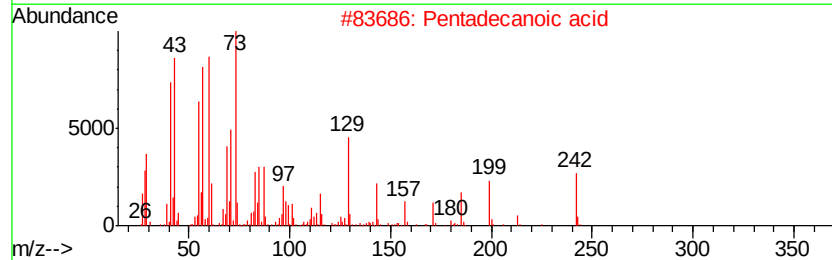
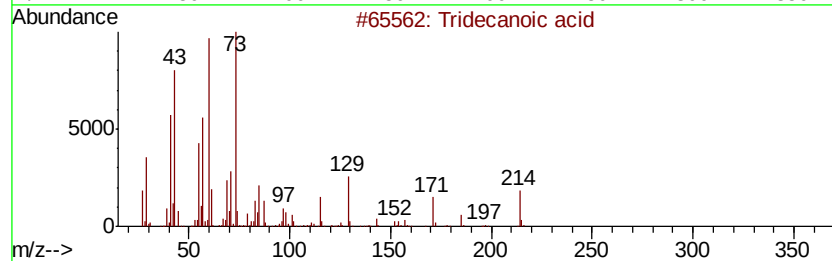
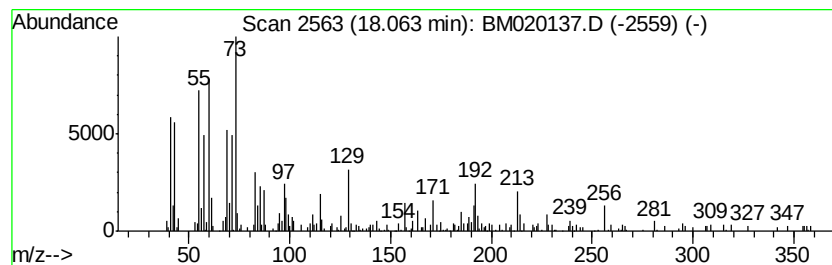
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	2.15 ng	219674	Phenanthrene-d10	17.18
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tridecanoic acid	214 C13H26O2	000638-53-9 95
2		Pentadecanoic acid	242 C15H30O2	001002-84-2 93
3		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 90
4		Tetradecanoic acid	228 C14H28O2	000544-63-8 58
5		Undecanoic acid	186 C11H22O2	000112-37-8 53



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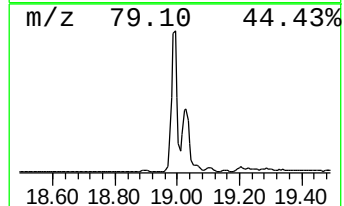
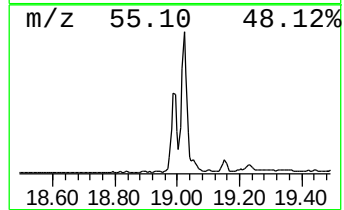
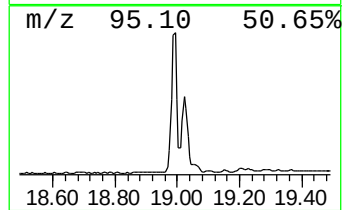
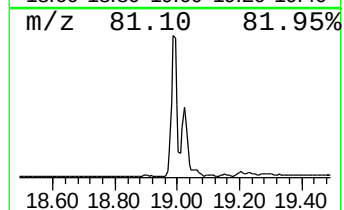
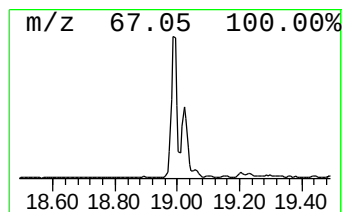
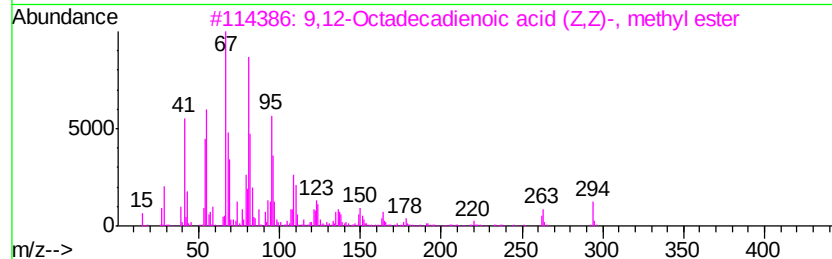
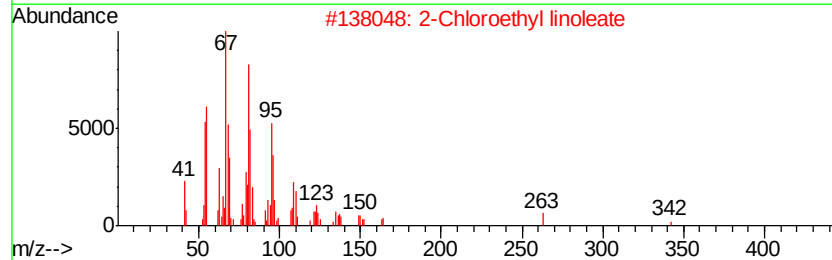
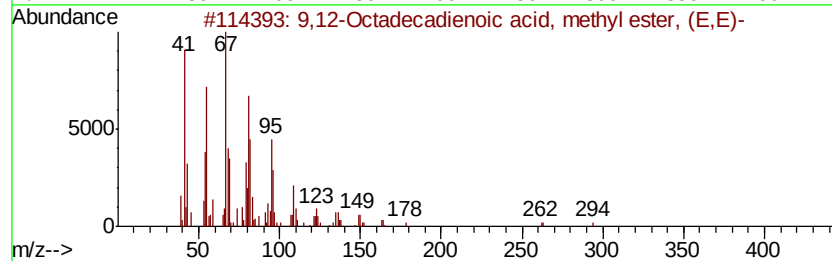
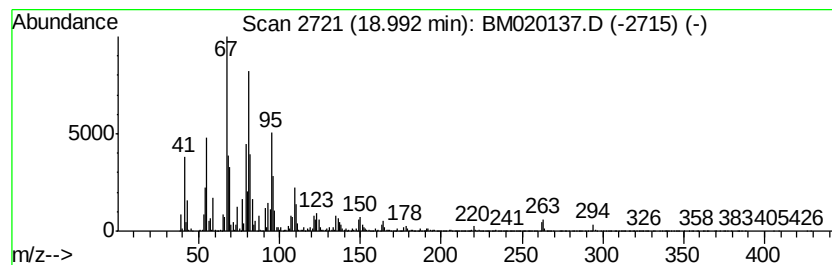
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.99	78.49 ng	8014150	Phenanthrene-d10	17.18		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95	
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93	
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	91	
4	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	83	
5	7-Hexadecyne	222	C16H30	074685-28-2	81	



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SU-04-050219-B

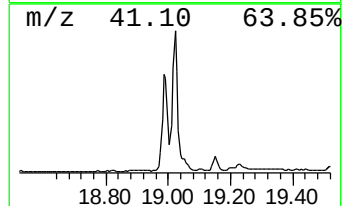
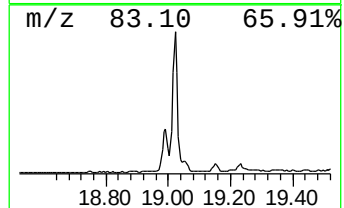
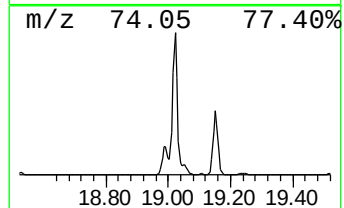
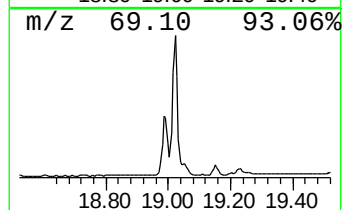
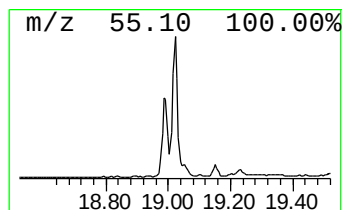
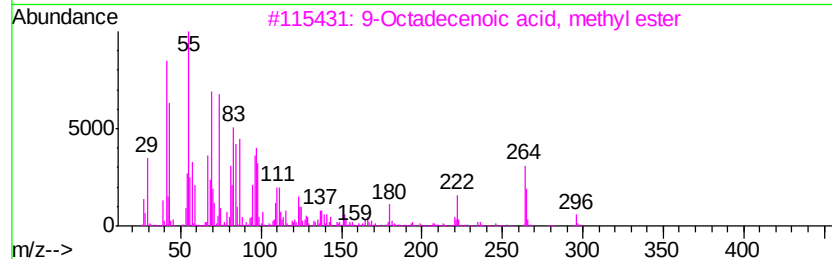
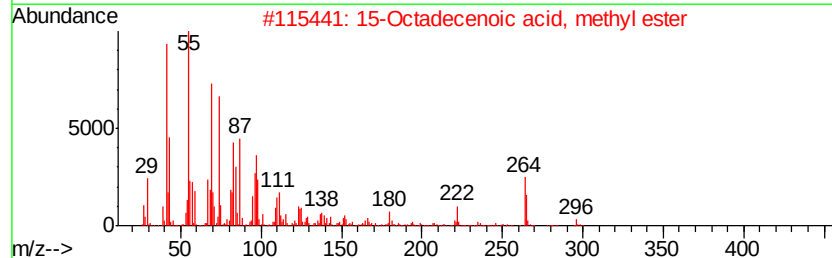
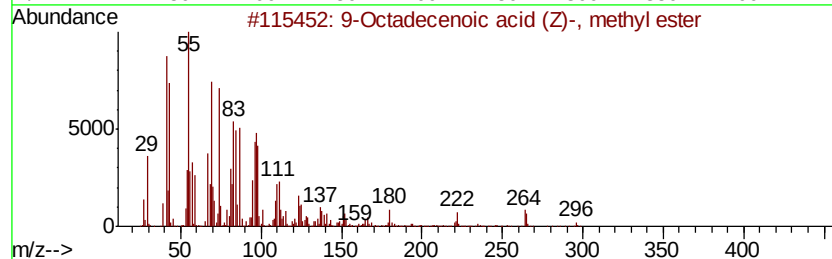
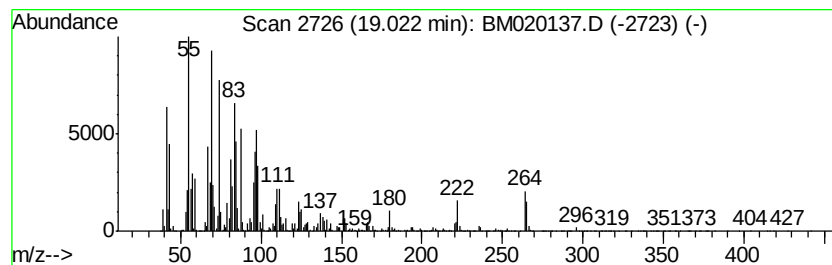
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	103.43 ng	10561100	Phenanthrene-d10	17.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3		9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4		11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050619\
Data File : BM020137.D
Acq On : 06 May 2019 16:00
Operator : JU/SJ
Sample : K2647-03 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

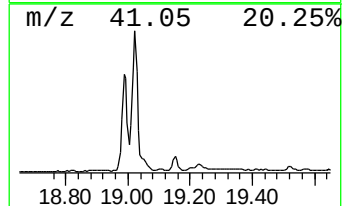
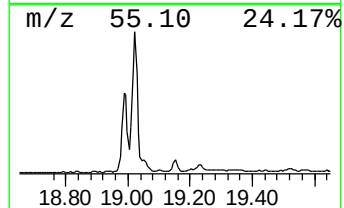
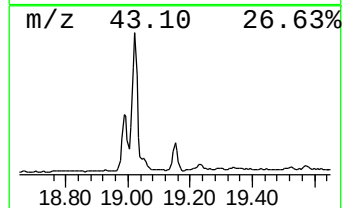
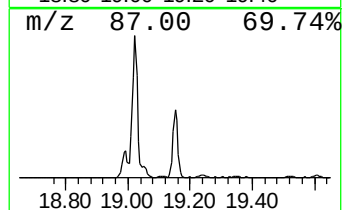
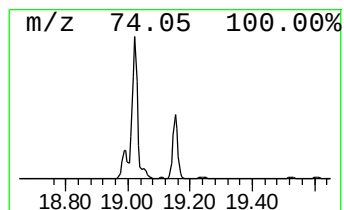
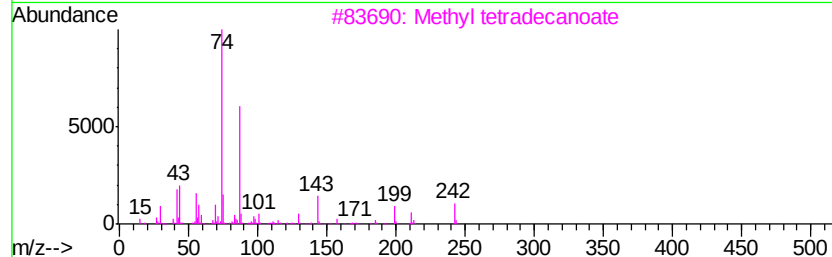
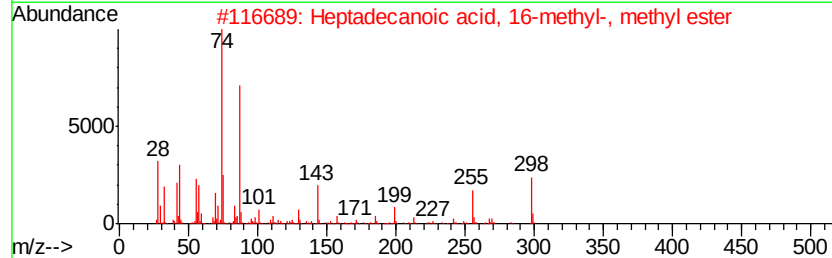
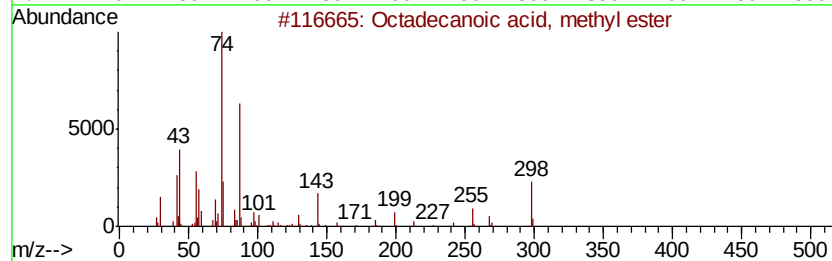
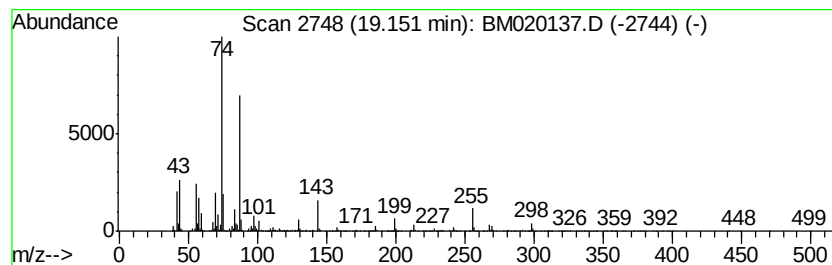
Instrument :
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ClientSampleId :
SU-04-050219-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.15	9.78 ng	998122	Phenanthrene-d10		17.18
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050619\
Data File : BM020137.D
Acq On : 06 May 2019 16:00
Operator : JU/SJ
Sample : K2647-03 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-04-050219-B

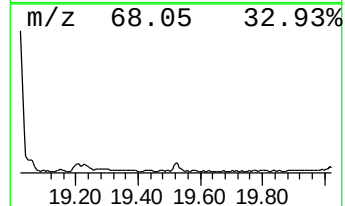
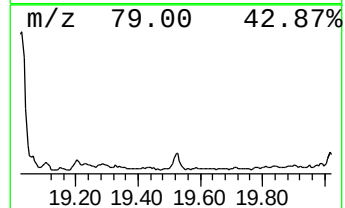
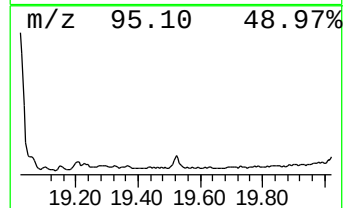
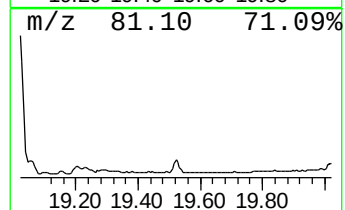
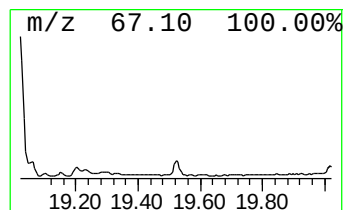
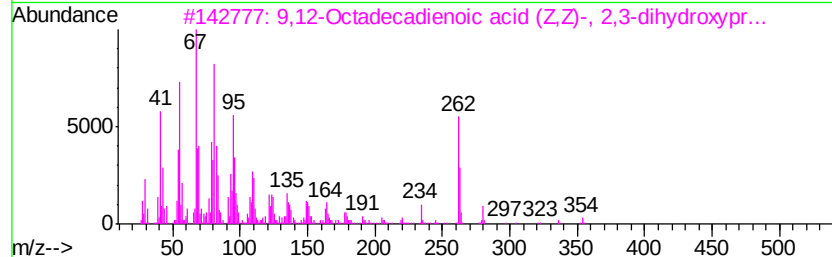
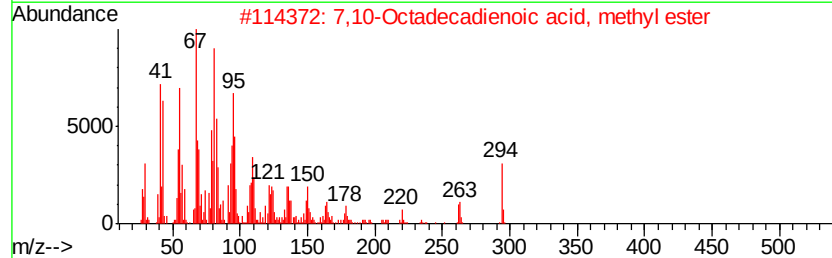
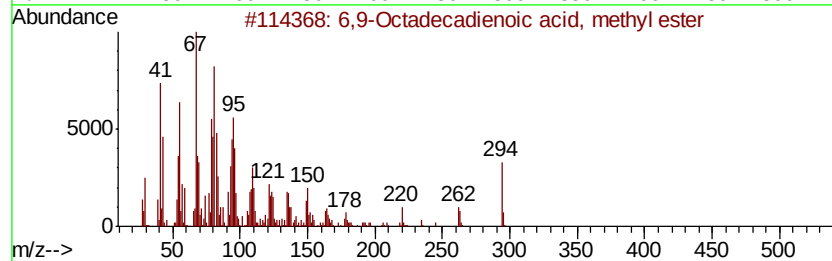
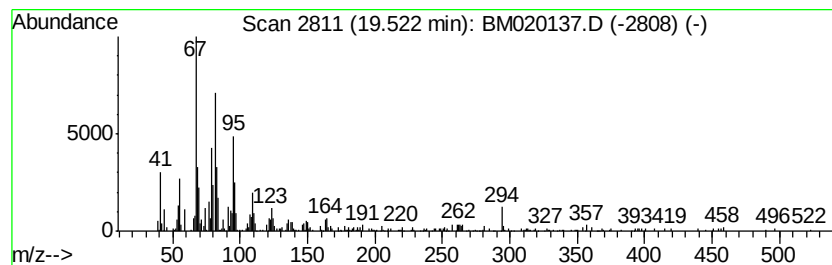
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 6,9-Octadecadienoic acid, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	2.78 ng	348043	Chrysene-d12	21.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6,9-Octadecadienoic acid, methyl...	294	C19H34O2	056599-55-4	89
2		7,10-Octadecadienoic acid, methyl...	294	C19H34O2	056554-24-6	89
3		9,12-Octadecadienoic acid (Z,Z)-...	354	C21H38O4	002277-28-3	87
4		1,E-11,Z-13-Octadecatriene	248	C18H32	080625-36-1	86
5		9,11-Octadecadienoic acid, methyl...	294	C19H34O2	013038-47-6	84



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM050619\
Data File : BM020137.D
Acq On : 06 May 2019 16:00
Operator : JU/SJ
Sample : K2647-03 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-04-050219-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Heptadecane	16.13	2.4	ng	240335	4	17.18	2042160	20.0
Pentadecanoic aci...	17.84	25.2	ng	2577480	4	17.18	2042160	20.0
Tridecanoic acid	18.06	2.1	ng	219674	4	17.18	2042160	20.0
9,12-Octadecadien...	18.99	78.5	ng	8014150	4	17.18	2042160	20.0
9-Octadecenoic ac...	19.02	103.4	ng	10561100	4	17.18	2042160	20.0
Octadecanoic acid...	19.15	9.8	ng	998122	4	17.18	2042160	20.0
6,9-Octadecadieno...	19.52	2.8	ng	348043	5	21.37	2500680	20.0