

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
 Data File : BF097014.D
 Acq On : 25 Jul 2017 4:40
 Operator : SJ/JU
 Sample : I4358-01 5X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-072017

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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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	4.646	466	469	476	rBV	53105	64668	2.13%	0.376%
2	5.116	545	549	563	rBV	601809	666427	21.91%	3.873%
3	6.175	725	729	745	rBV	688416	675749	22.22%	3.927%
4	6.287	745	748	756	rVB	796618	658966	21.67%	3.829%
5	6.516	783	787	791	rBV	1030086	891940	29.33%	5.183%
6	6.669	809	813	822	rVB	586286	483432	15.89%	2.809%
7	7.075	879	882	891	rBV	431488	371723	12.22%	2.160%
8	7.798	1001	1005	1008	rBV	1338614	1064156	34.99%	6.184%
9	8.875	1184	1188	1191	rBV	706819	573270	18.85%	3.331%
10	9.545	1297	1302	1305	rBV	966021	897193	29.50%	5.214%
11	9.969	1367	1374	1377	rBV	93322	81776	2.69%	0.475%
12	10.328	1432	1435	1441	rBV	267151	231142	7.60%	1.343%
13	10.569	1474	1476	1479	rBV	45457	35180	1.16%	0.204%
14	11.016	1548	1552	1555	rBV	859273	720229	23.68%	4.185%
15	11.039	1555	1556	1561	rVB	59876	35618	1.17%	0.207%
16	11.357	1604	1610	1614	rBV2	122928	129879	4.27%	0.755%
17	11.439	1620	1624	1627	rVB	1427660	1264029	41.56%	7.346%
18	11.575	1644	1647	1653	rBV2	123264	127041	4.18%	0.738%
19	11.839	1690	1692	1696	rVB	40663	34628	1.14%	0.201%
20	12.116	1735	1739	1741	rBV	1211562	1207263	39.69%	7.016%
21	12.139	1741	1743	1751	rVV	2844524	3041469	100.00%	17.675%
22	12.227	1754	1758	1761	rVB2	869670	803218	26.41%	4.668%
23	12.275	1761	1766	1774	rBV	109874	151294	4.97%	0.879%
24	12.445	1791	1795	1802	rVB	181564	220227	7.24%	1.280%
25	12.598	1818	1821	1825	rVB	487221	410312	13.49%	2.384%
26	12.816	1854	1858	1861	rVB5	41317	58418	1.92%	0.339%
27	12.869	1861	1867	1875	rVB5	105830	157756	5.19%	0.917%
28	12.945	1878	1880	1883	rBV	47094	47857	1.57%	0.278%
29	13.051	1894	1898	1902	rBV	135753	133000	4.37%	0.773%
30	13.145	1910	1914	1917	rBV4	30787	44125	1.45%	0.256%
31	13.369	1948	1952	1955	rBV3	67286	96438	3.17%	0.560%
32	13.522	1975	1978	1980	rBV2	46256	42806	1.41%	0.249%
33	13.645	1994	1999	2001	rVV	788757	854438	28.09%	4.965%
34	13.669	2001	2003	2005	rVB	60137	52274	1.72%	0.304%

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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 >
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35	13.839	2029	2032	2036	rBV3	41512	42926	1.41%	0.249%
36	14.145	2081	2084	2087	rBV	56950	73851	2.43%	0.429%
37	14.433	2131	2133	2137	rBV	66465	81280	2.67%	0.472%
38	14.727	2181	2183	2187	rVB	83602	72356	2.38%	0.420%
39	14.998	2225	2229	2234	rBV	542570	609588	20.04%	3.542%

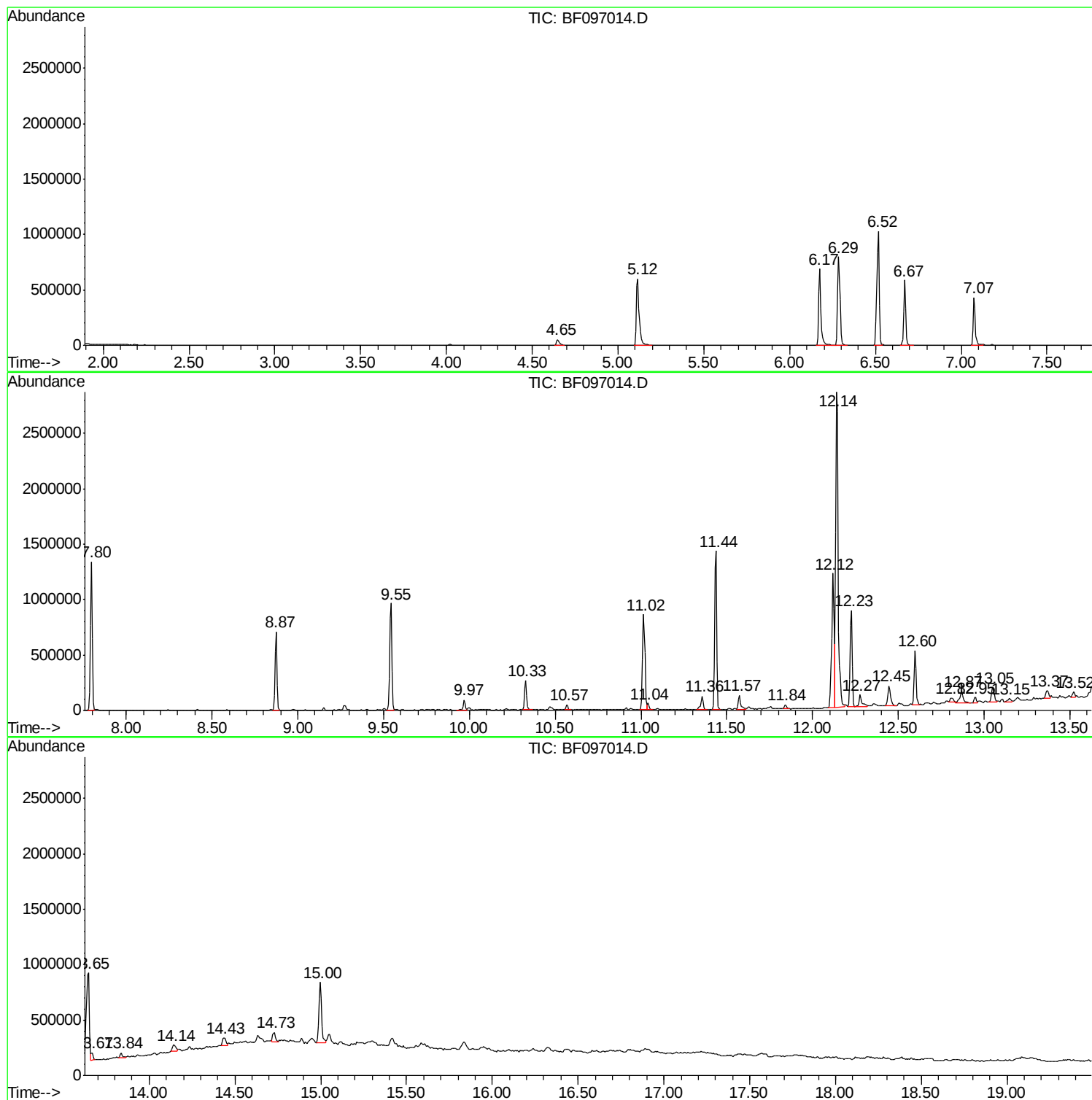
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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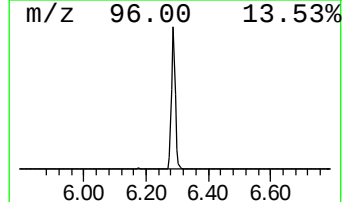
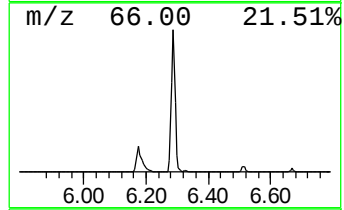
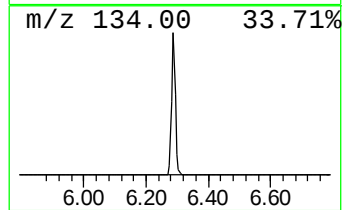
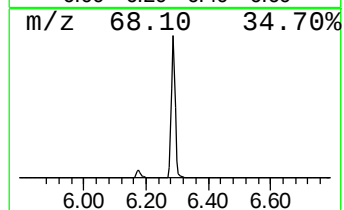
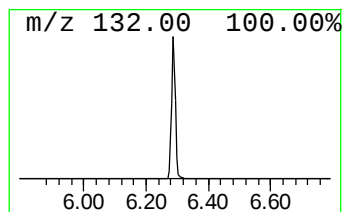
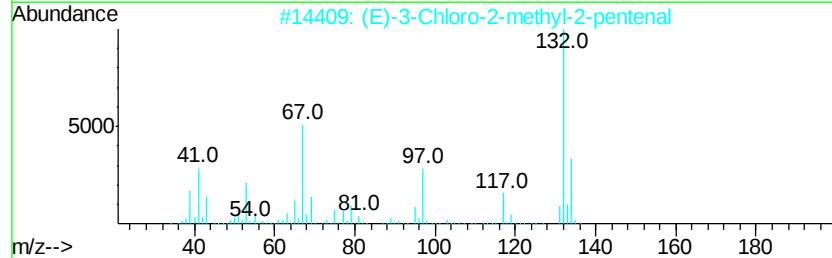
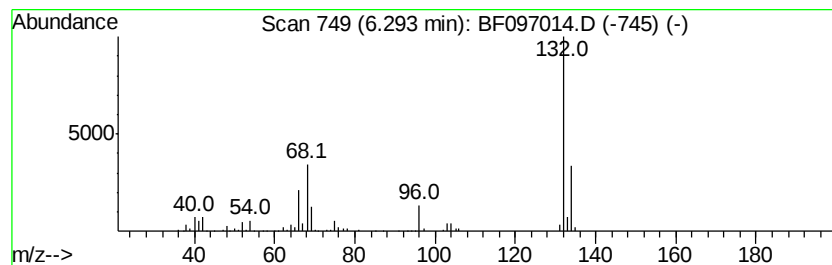
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	14.78 ng	658966	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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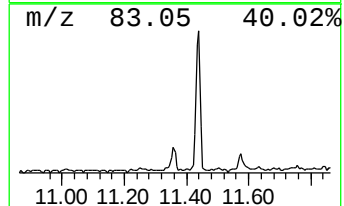
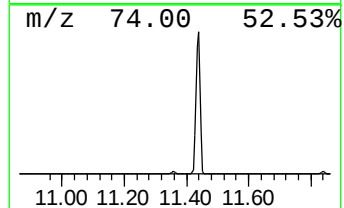
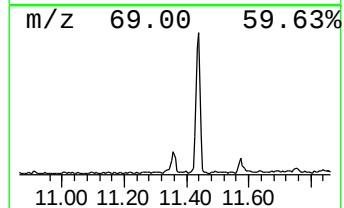
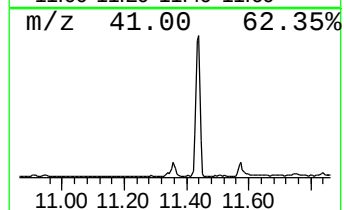
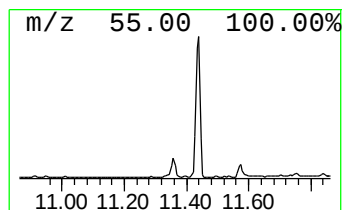
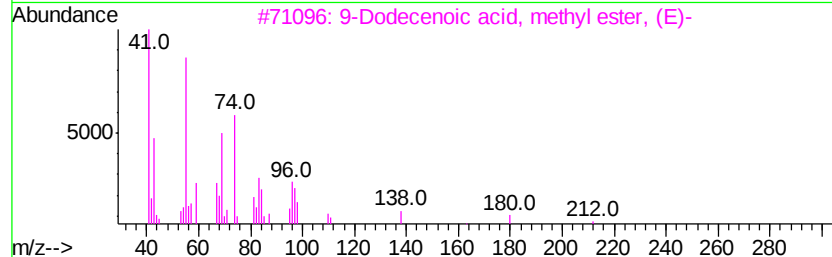
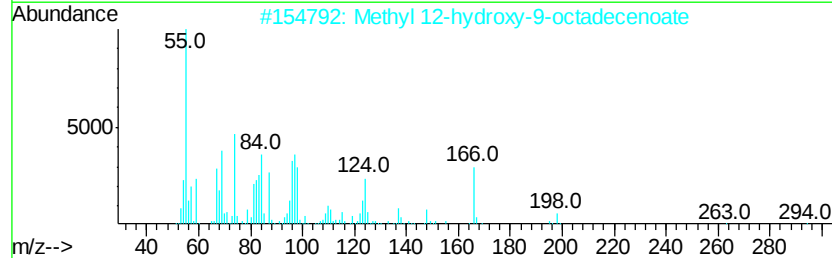
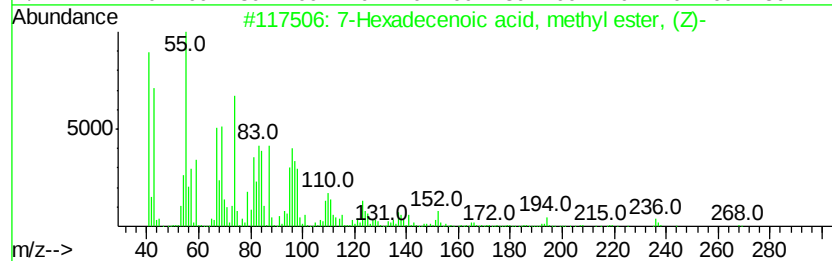
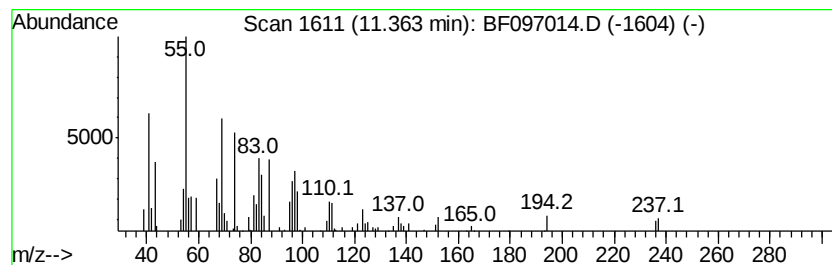
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Peak Number 3 7-Hexadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	3.61 ng	129879	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	74
2		Methyl 12-hydroxy-9-octadecenoate	312	C19H36O3	1000336-28-8	72
3		9-Dodecenoic acid, methyl ester,...	212	C13H24O2	055030-26-7	53
4		Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-30-8	52
5		Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-31-9	50



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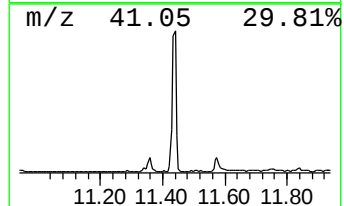
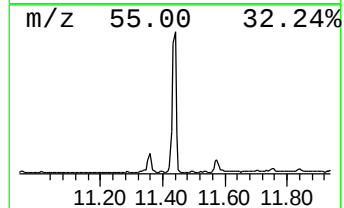
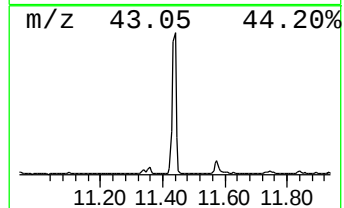
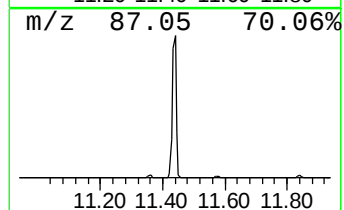
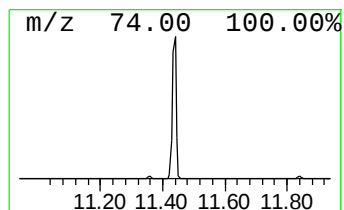
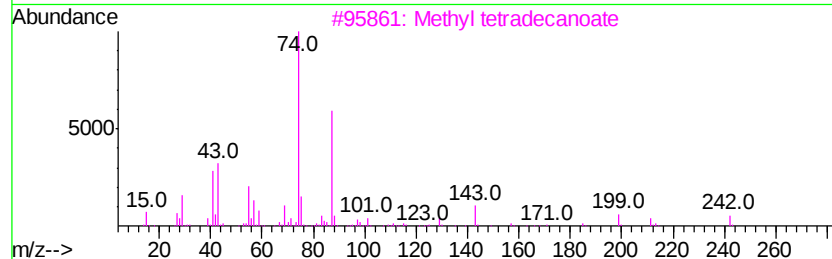
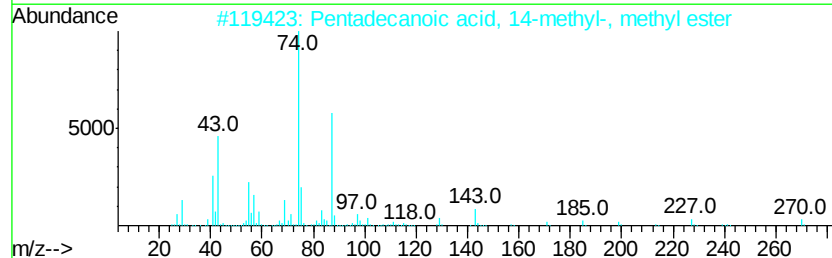
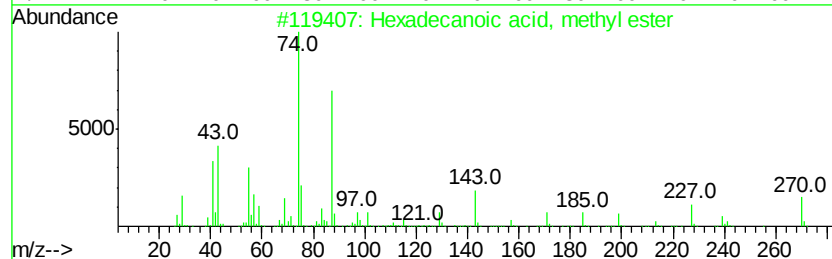
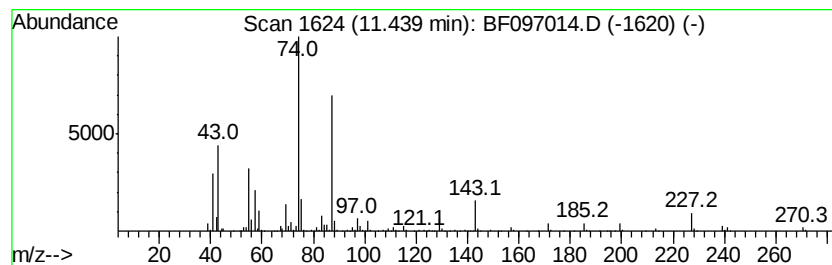
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	35.10 ng	1264030	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	87



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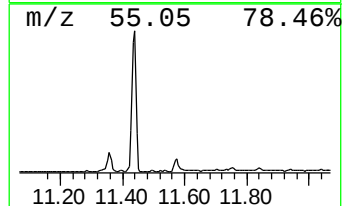
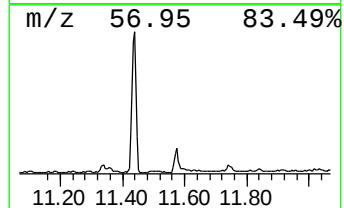
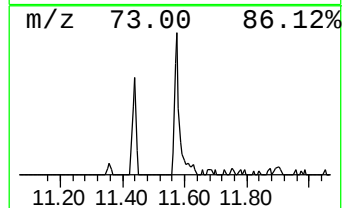
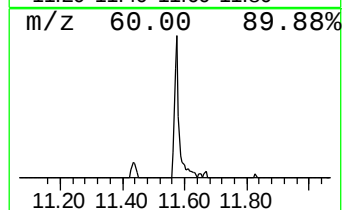
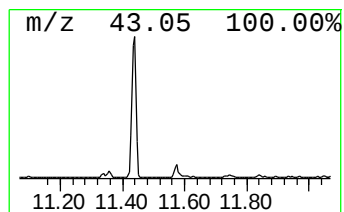
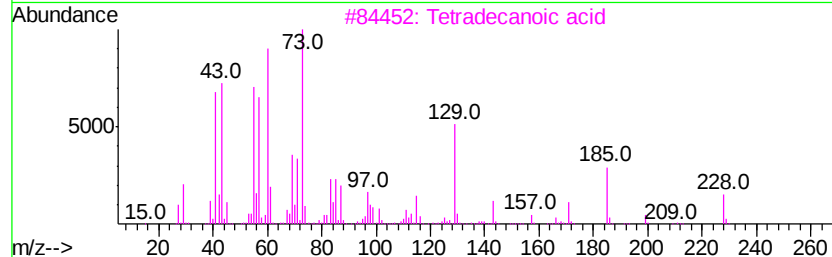
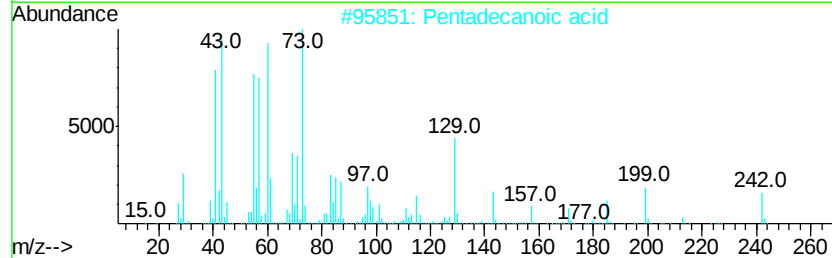
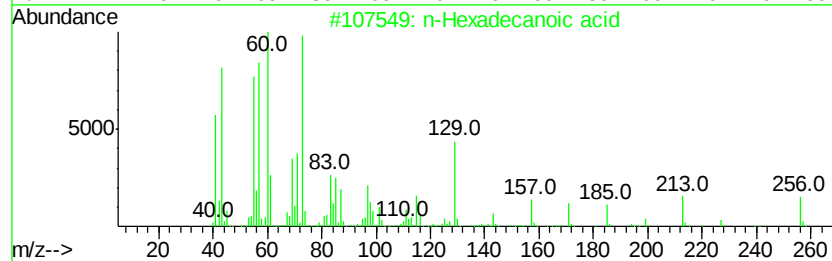
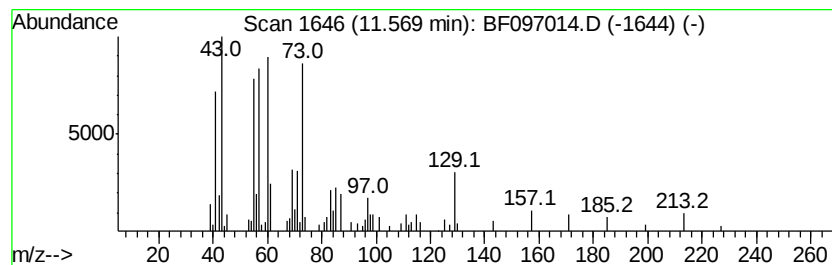
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	3.53 ng	127041	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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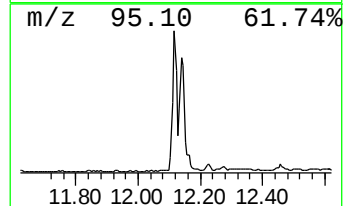
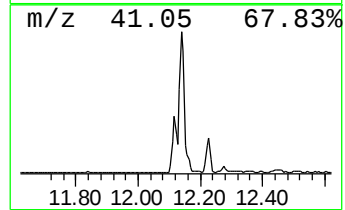
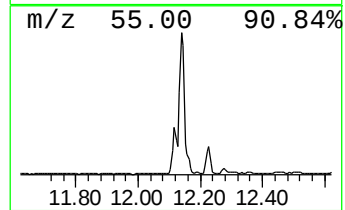
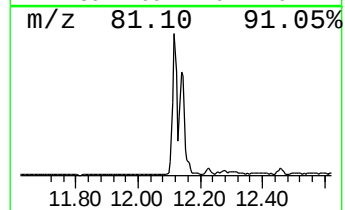
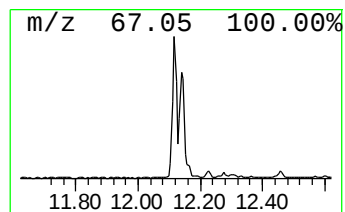
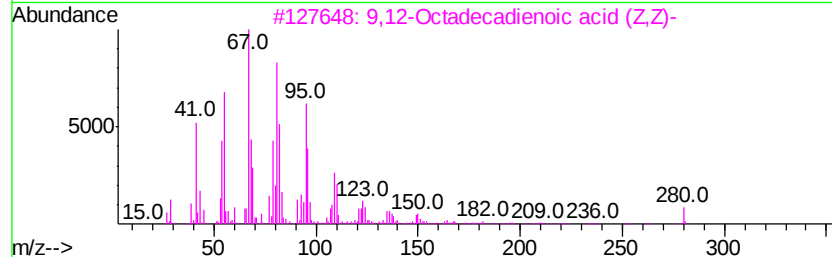
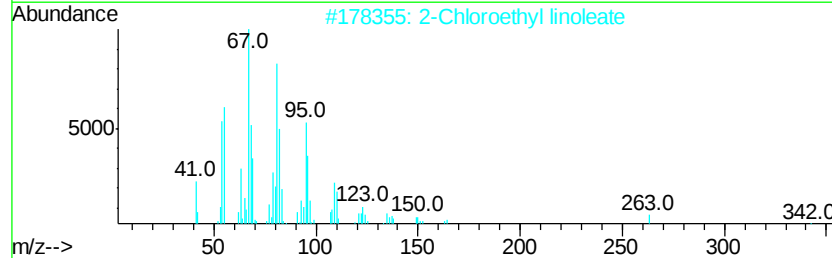
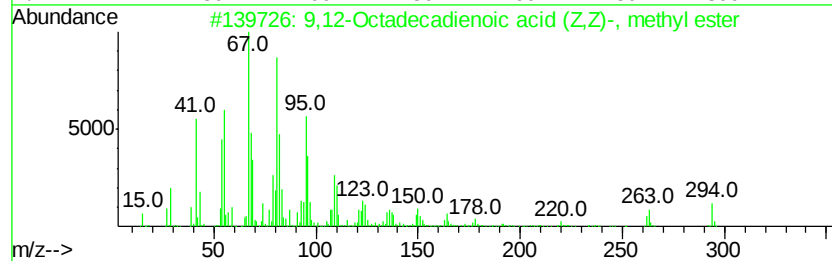
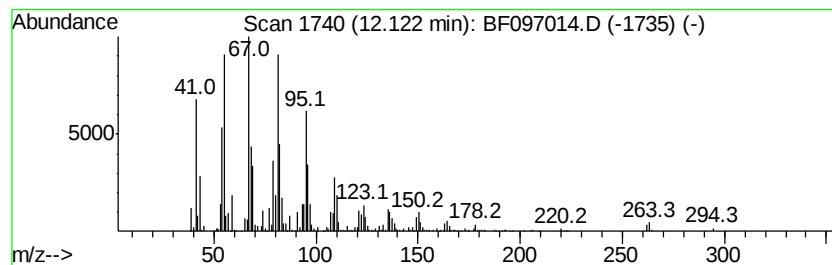
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Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	33.52 ng	1207260	Phenanthrene-d10	11.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
3		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	93
5		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	91



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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-072017

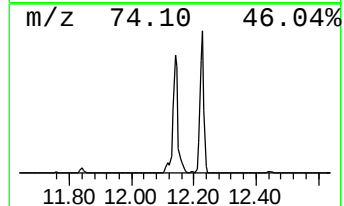
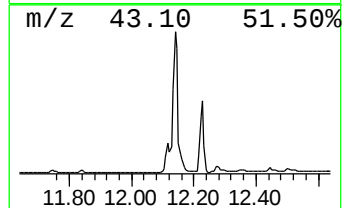
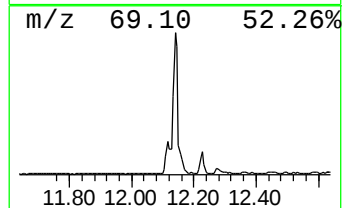
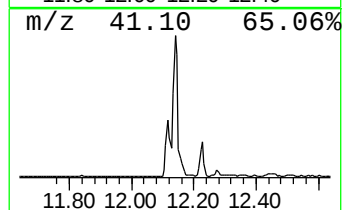
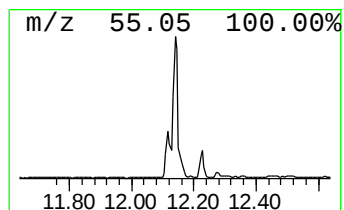
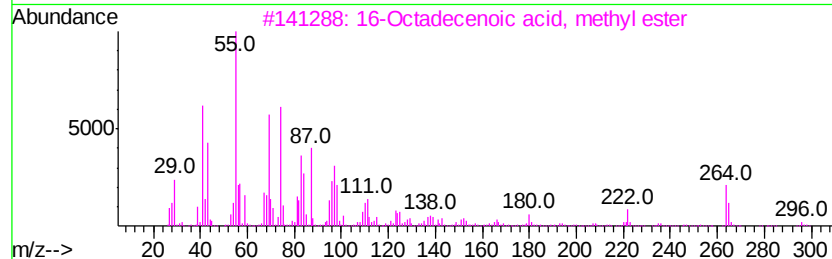
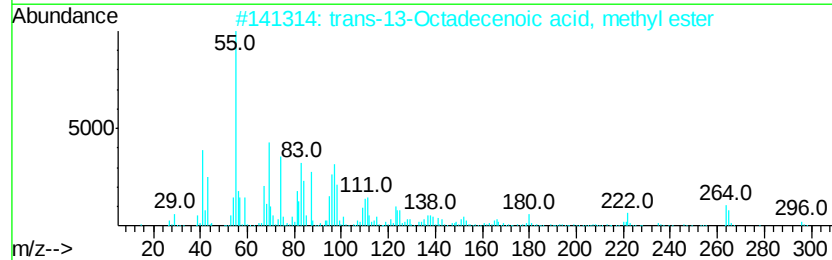
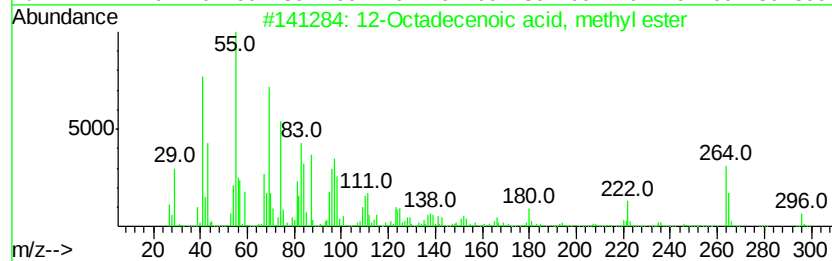
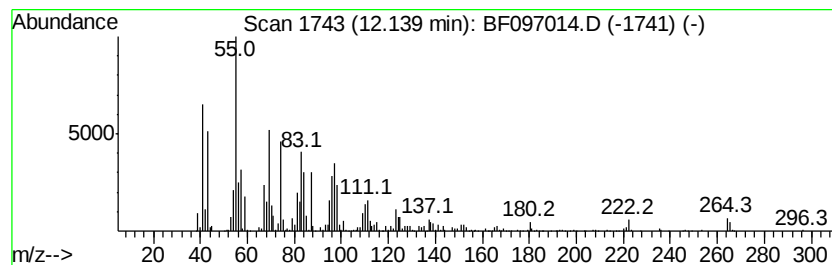
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 12-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	84.46 ng	3041470	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2		trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	96
3		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
4		6-Octadecenoic acid, methyl ester	296	C19H36O2	002777-58-4	95
5		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF097014.D
Acq On : 25 Jul 2017 4:40
Operator : SJ/JU
Sample : I4358-01 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

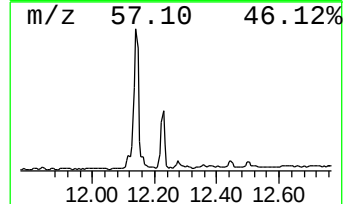
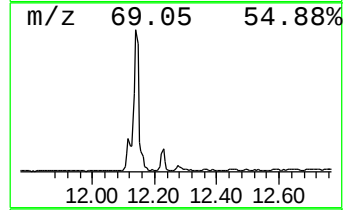
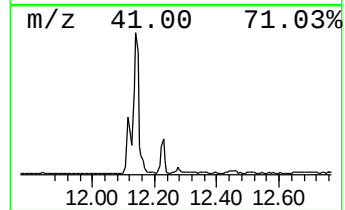
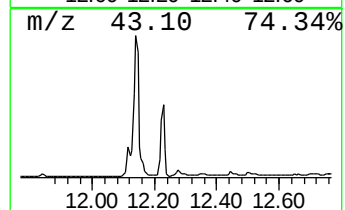
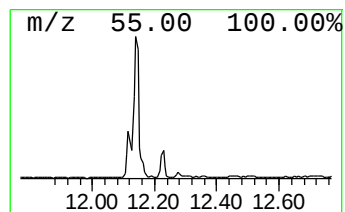
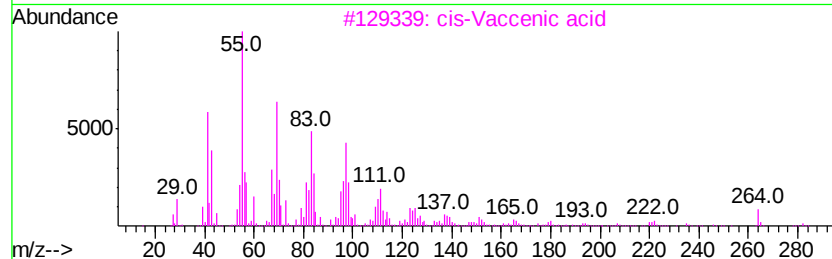
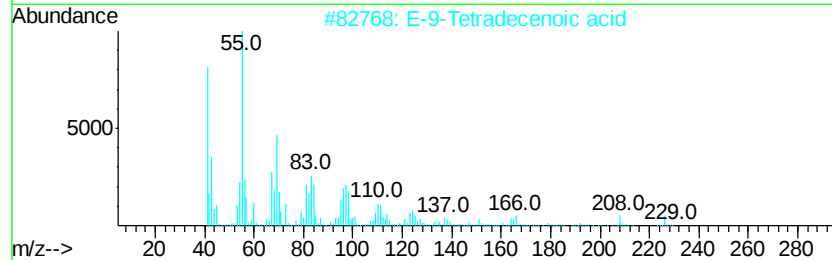
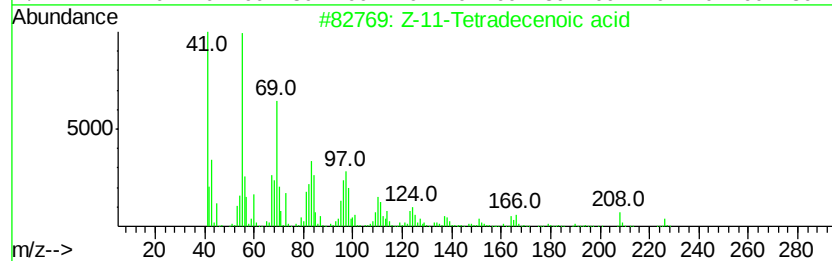
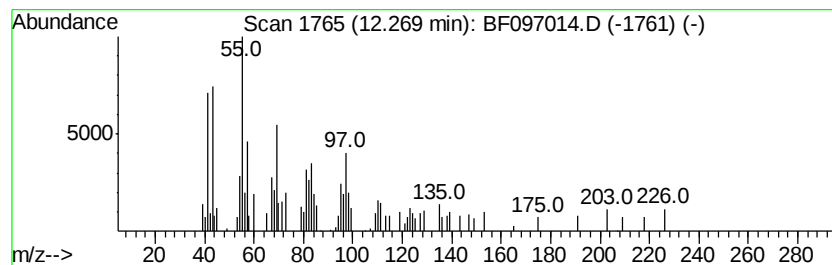
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Z-11-Tetradecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.27	4.20 ng	151294	Phenanthrene-d10	11.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	95
2	E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	91
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
5	Oleic Acid	282	C18H34O2	000112-80-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097014.D
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Operator : SJ/JU
Sample : I4358-01 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

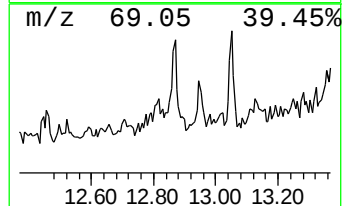
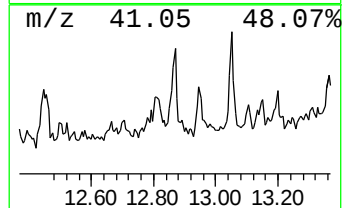
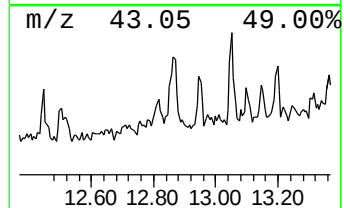
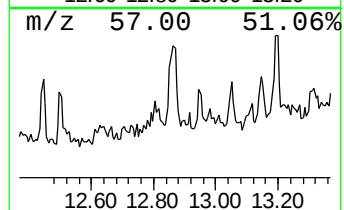
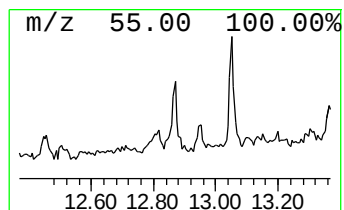
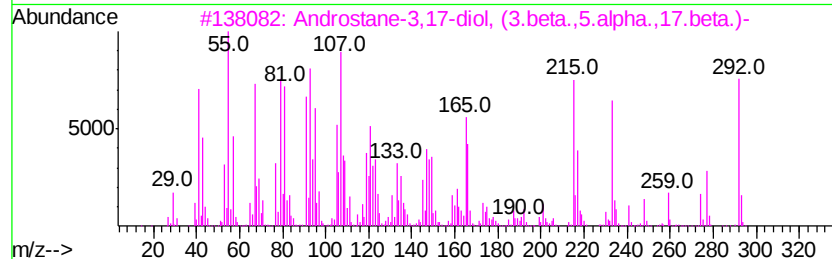
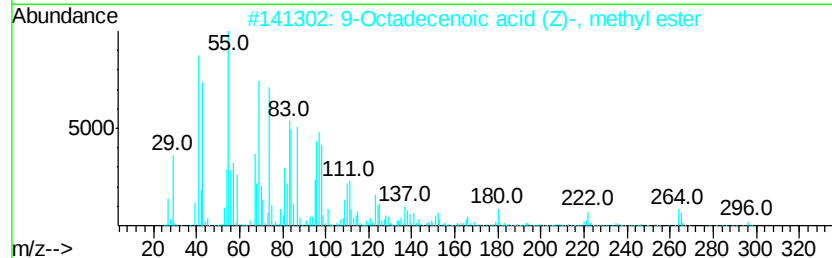
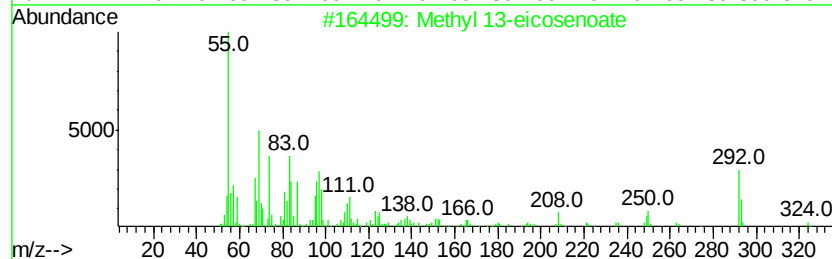
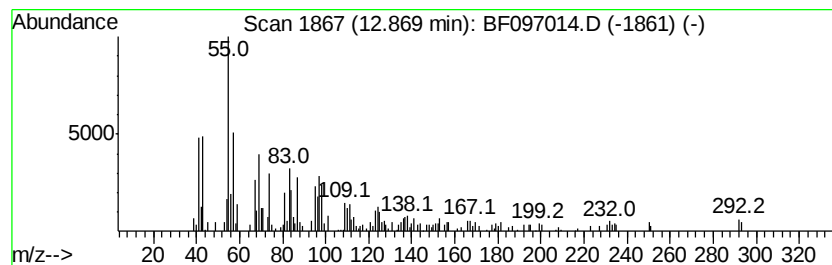
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Methyl 13-eicosenoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.87	3.69 ng	157756	Chrysene-d12	13.65		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	68
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	62
3		Androstane-3,17-diol, (3.beta.,5...	292	C19H32O2	000571-20-0	56
4		Butyl 9-tetradecenoate	282	C18H34O2	1000336-51-4	49
5		9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
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Operator : SJ/JU
Sample : I4358-01 5X
Misc :
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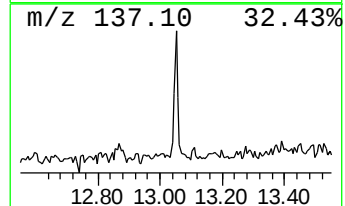
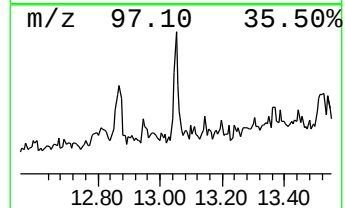
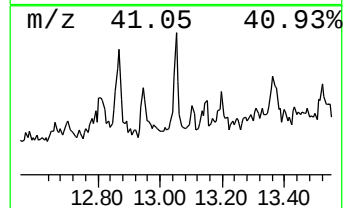
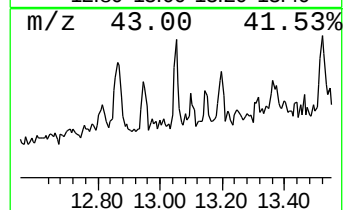
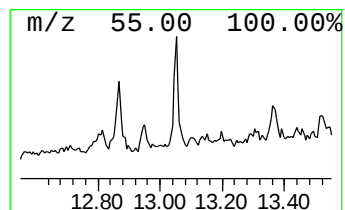
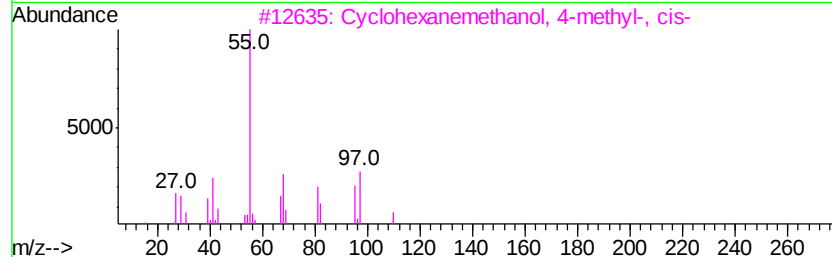
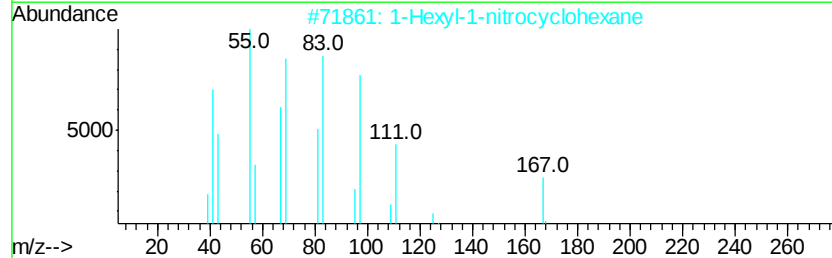
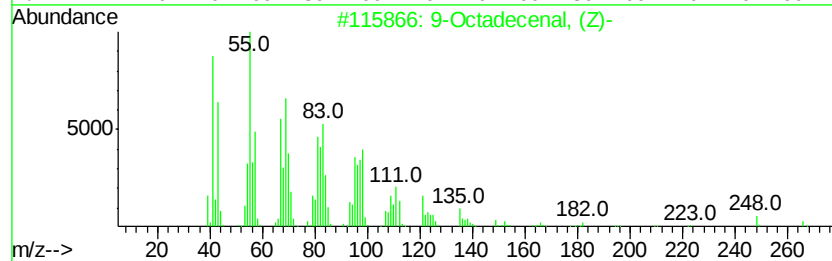
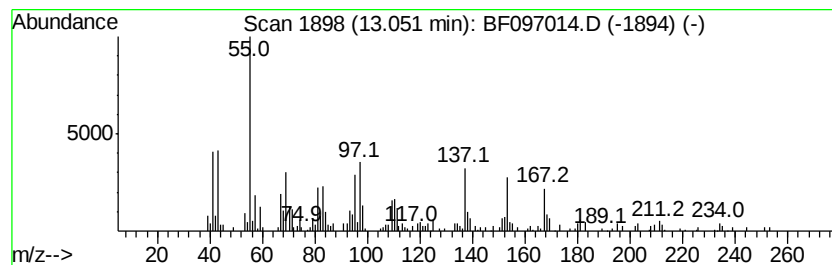
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown13.05 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.05	3.11 ng	133000	Chrysene-d12	13.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenal, (Z)-	266	C18H34O	002423-10-1	16
2	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	14
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	14
4	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	14
5	Cyclododecanemethanol	198	C13H26O	001892-12-2	12



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
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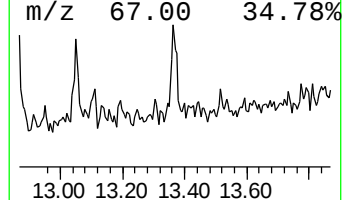
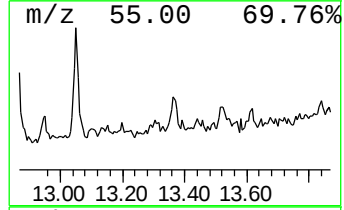
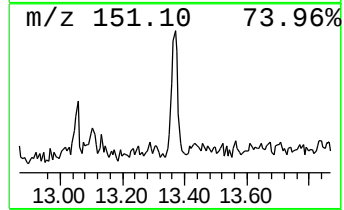
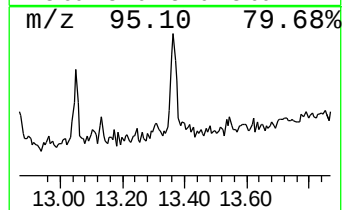
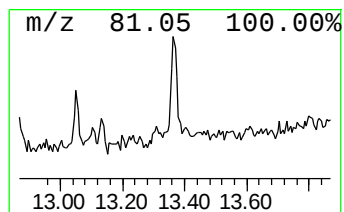
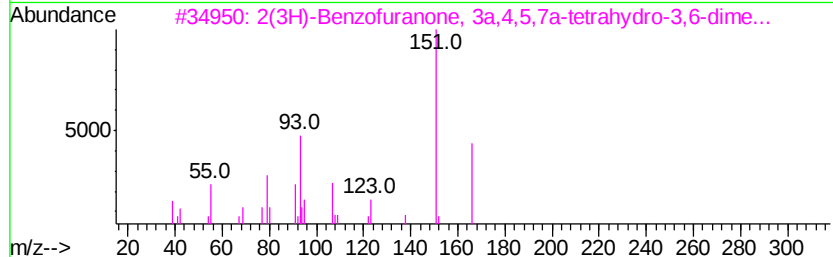
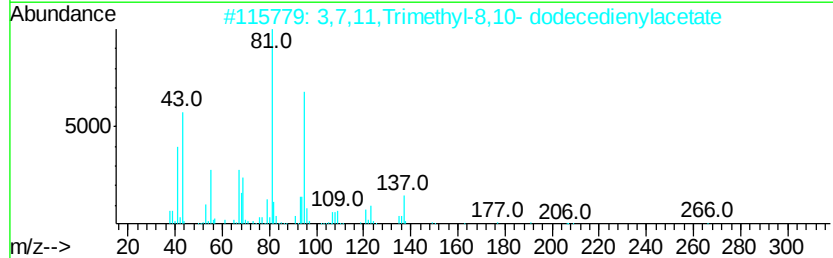
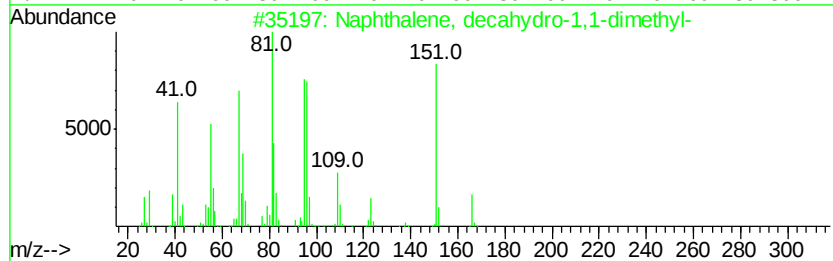
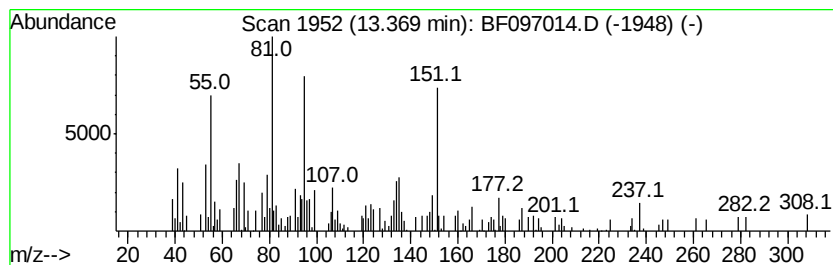
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown13.37 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	2.26 ng	96438	Chrysene-d12	13.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-1,1-dimet...	166	C12H22	035431-04-0	46
2		3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	30
3		2(3H)-Benzofuranone, 3a,4,5,7a-t...	166	C10H14O2	1000360-45-0	25
4		Pentacyclo[6.3.0.0(2,7).0(4,11)...]	160	C11H12O	069649-19-0	25
5		Phenol, 2,6-dimethyl-4-nitroso-	151	C8H9NO2	013331-93-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
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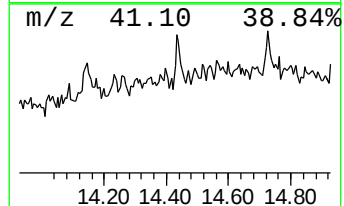
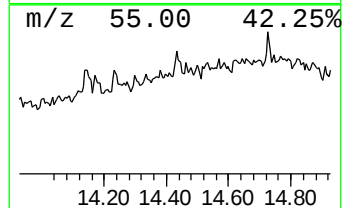
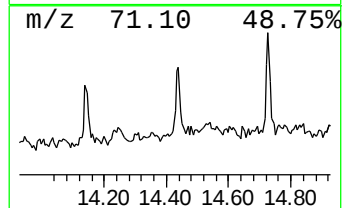
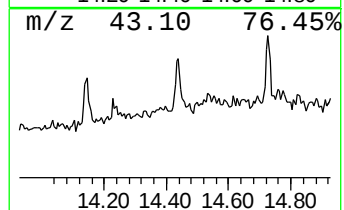
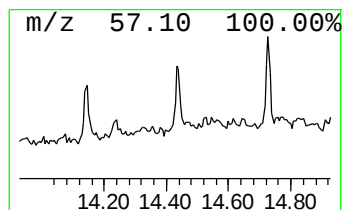
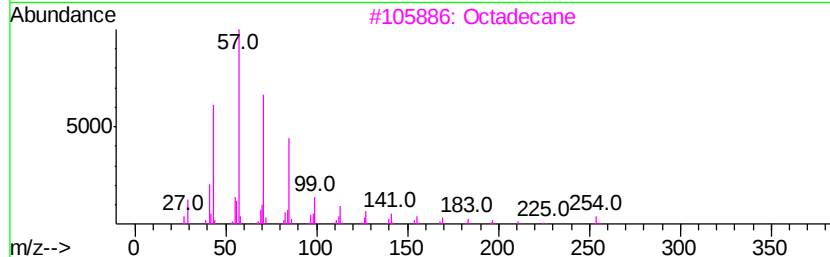
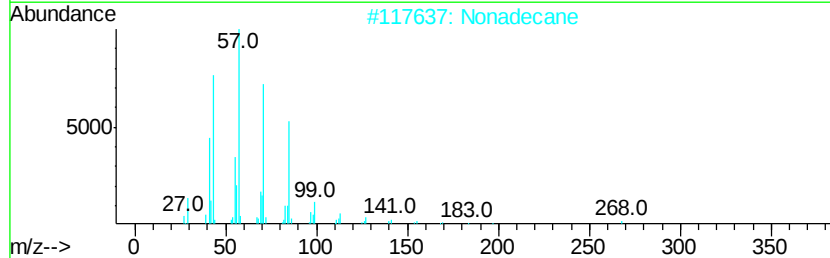
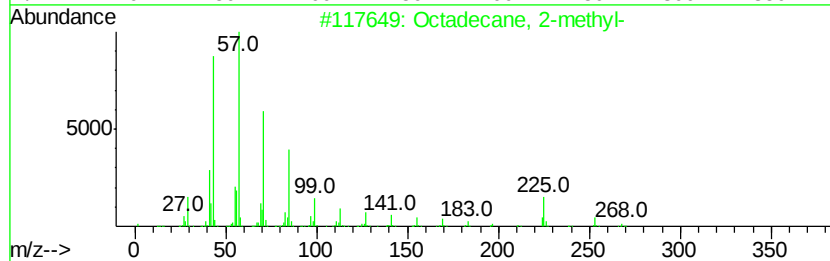
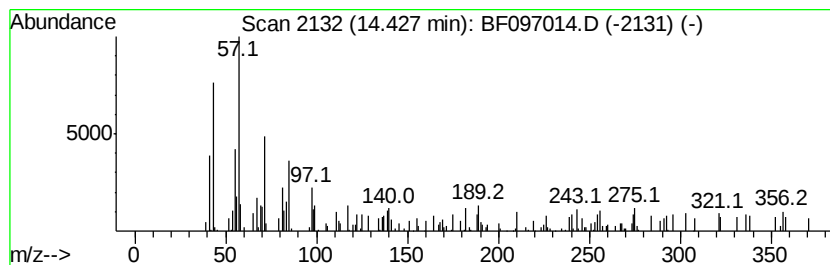
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.67 ng	81280	Perylene-d12	15.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	70
2		Nonadecane	268	C19H40	000629-92-5	70
3		Octadecane	254	C18H38	000593-45-3	64
4		Heptadecane	240	C17H36	000629-78-7	64
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	62



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Misc :
ALS Vial : 24 Sample Multiplier: 1

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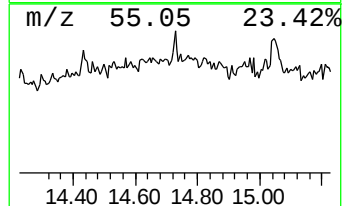
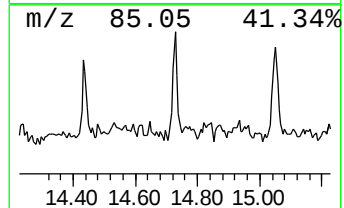
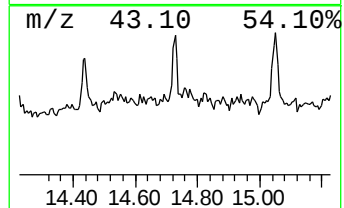
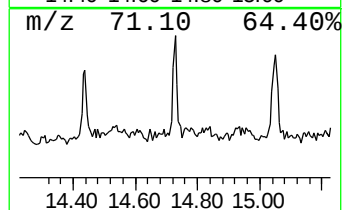
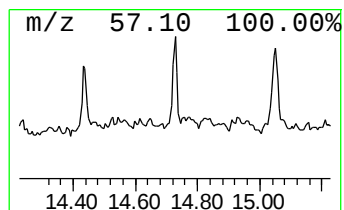
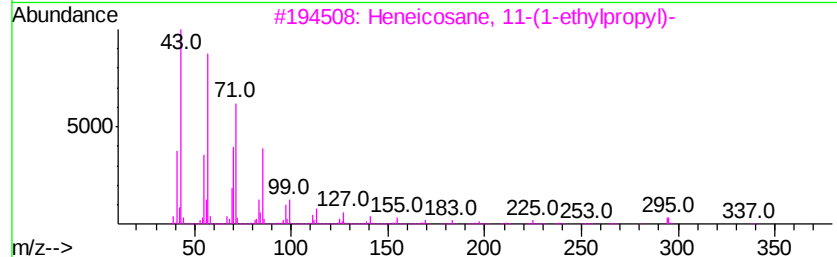
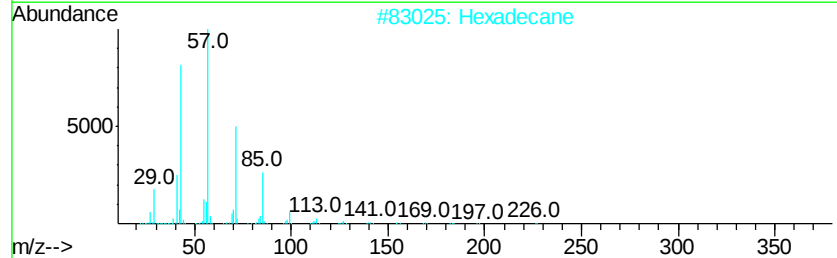
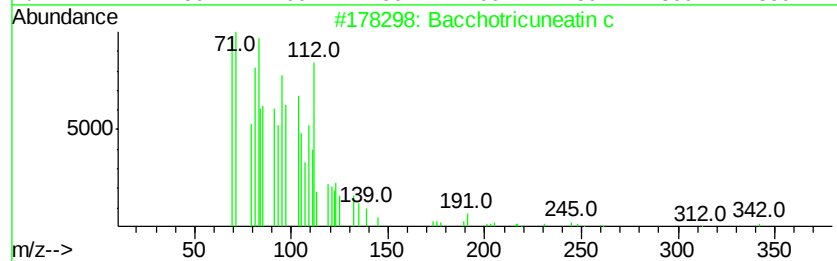
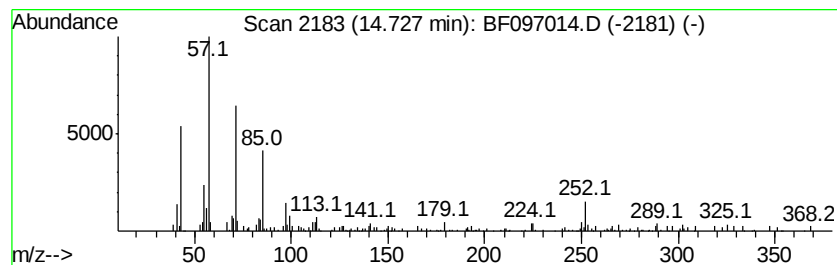
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Bacchotricuneatin c Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.37 ng	72356	Perylene-d12	15.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	97
2		Hexadecane	226	C16H34	000544-76-3	70
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	64
4		Tetracosane	338	C24H50	000646-31-1	62
5		Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
 Data File : BF097014.D
 Acq On : 25 Jul 2017 4:40
 Operator : SJ/JU
 Sample : I4358-01 5X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-072017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.29	6.29	14.8	ng	658966	1	6.52	891940	20.0
7-Hexadecenoic ac...	11.36	3.6	ng	129879	4	11.02	720229	20.0
Hexadecanoic acid...	11.44	35.1	ng	1264030	4	11.02	720229	20.0
n-Hexadecanoic acid	11.57	3.5	ng	127041	4	11.02	720229	20.0
9,12-Octadecadien...	12.12	33.5	ng	1207260	4	11.02	720229	20.0
12-Octadecenoic a...	12.14	84.5	ng	3041470	4	11.02	720229	20.0
Z-11-Tetradeceno...	12.27	4.2	ng	151294	4	11.02	720229	20.0
Methyl 13-eicosen...	12.87	3.7	ng	157756	5	13.65	854438	20.0
unknown13.05	13.05	3.1	ng	133000	5	13.65	854438	20.0
unknown13.37	13.37	2.3	ng	96438	5	13.65	854438	20.0
Octadecane, 2-met...	14.43	2.7	ng	81280	6	15.00	609588	20.0
Bacchotricuneatin c	14.73	2.4	ng	72356	6	15.00	609588	20.0