

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
 Data File : BF106352.D
 Acq On : 12 Jun 2018 18:43
 Operator : JU/SJ
 Sample : J3415-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-35COMP

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_F\METHODS\8270-BF061118.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	5.207	484	488	497	rVB	244141	290972	1.57%	0.344%
2	5.601	550	555	558	rBV	2865865	2997365	16.20%	3.547%
3	6.595	719	724	727	rBV	2977218	2900861	15.68%	3.433%
4	6.742	745	749	752	rBV	3220000	2925198	15.81%	3.462%
5	6.972	785	788	792	rVB	1116362	872146	4.71%	1.032%
6	7.131	811	815	818	rBV	2733176	2320578	12.54%	2.746%
7	7.531	879	883	887	rBV	1901410	1869476	10.10%	2.212%
8	8.254	1002	1006	1009	rBV	1207963	952033	5.15%	1.127%
9	9.330	1184	1189	1192	rBV	2870068	2548529	13.77%	3.016%
10	9.583	1229	1232	1239	rVB	321386	259081	1.40%	0.307%
11	9.719	1252	1255	1258	rBV	512646	388603	2.10%	0.460%
12	10.013	1301	1305	1308	rBV	1100856	914645	4.94%	1.082%
13	10.430	1369	1376	1379	rBV	253921	235750	1.27%	0.279%
14	10.801	1436	1439	1443	rBV	1931108	1660034	8.97%	1.965%
15	10.901	1453	1456	1462	rBV	251815	319446	1.73%	0.378%
16	11.007	1471	1474	1477	rVB	408073	330217	1.78%	0.391%
17	11.501	1555	1558	1561	rBV	1072058	1002486	5.42%	1.186%
18	11.783	1604	1606	1608	rBV2	213594	214422	1.16%	0.254%
19	11.807	1608	1610	1614	rVB	887434	661106	3.57%	0.782%
20	11.895	1619	1625	1628	rBV	6635942	10142083	54.81%	12.003%
21	12.030	1642	1648	1654	rBV2	203974	269187	1.45%	0.319%
22	12.207	1676	1678	1682	rVB	342117	272755	1.47%	0.323%
23	12.289	1688	1692	1697	rBV	415725	378783	2.05%	0.448%
24	12.601	1736	1745	1747	rBV2	6530367	18503738	100.00%	21.898%
25	12.695	1758	1761	1764	rVB	6038449	6369576	34.42%	7.538%
26	12.742	1767	1769	1771	rBV	301630	305400	1.65%	0.361%
27	12.795	1776	1778	1782	rVB2	224358	200904	1.09%	0.238%
28	12.918	1796	1799	1803	rVB	1058275	963175	5.21%	1.140%
29	12.971	1803	1808	1813	rVB4	404958	638733	3.45%	0.756%
30	13.036	1816	1819	1823	rVB3	248694	204276	1.10%	0.242%
31	13.101	1825	1830	1832	rBV	3223129	3014479	16.29%	3.567%
32	13.118	1832	1833	1836	rVV	445313	328769	1.78%	0.389%
33	13.165	1836	1841	1844	rVV	383592	483969	2.62%	0.573%
34	13.277	1851	1860	1863	rBV3	1042244	1894654	10.24%	2.242%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.330	1863	1869	1875	rVB	2450139	2940748	15.89%	3.480%
36	13.407	1878	1882	1884	rBV	1860168	1794592	9.70%	2.124%
37	13.424	1884	1885	1890	rVV3	697996	709960	3.84%	0.840%
38	13.465	1890	1892	1895	rVV2	629597	613024	3.31%	0.725%
39	13.518	1897	1901	1905	rVV3	665096	1122302	6.07%	1.328%
40	13.571	1907	1910	1912	rVV2	578120	711896	3.85%	0.842%
41	13.601	1912	1915	1920	rVV4	345782	591872	3.20%	0.700%
42	13.712	1930	1934	1936	rBV4	157122	232625	1.26%	0.275%
43	13.742	1936	1939	1942	rVV2	269812	346372	1.87%	0.410%
44	13.771	1942	1944	1949	rVV3	163130	223223	1.21%	0.264%
45	13.842	1951	1956	1961	rVB2	1409474	1968034	10.64%	2.329%
46	13.977	1977	1979	1983	rVB2	465631	418913	2.26%	0.496%
47	14.083	1993	1997	2001	rBV	1467419	1327975	7.18%	1.572%
48	14.165	2007	2011	2014	rBV	1271279	1141358	6.17%	1.351%
49	14.407	2050	2052	2059	rBV2	155018	204420	1.10%	0.242%
50	14.636	2088	2091	2093	rBV	198924	192342	1.04%	0.228%
51	14.665	2093	2096	2099	rBV2	230736	227021	1.23%	0.269%
52	14.730	2104	2107	2112	rBV	589800	585650	3.17%	0.693%
53	15.042	2157	2160	2163	rVB	202337	196192	1.06%	0.232%
54	15.318	2204	2207	2213	rBV	215769	265648	1.44%	0.314%
55	15.712	2270	2274	2286	rVB	669699	1050833	5.68%	1.244%

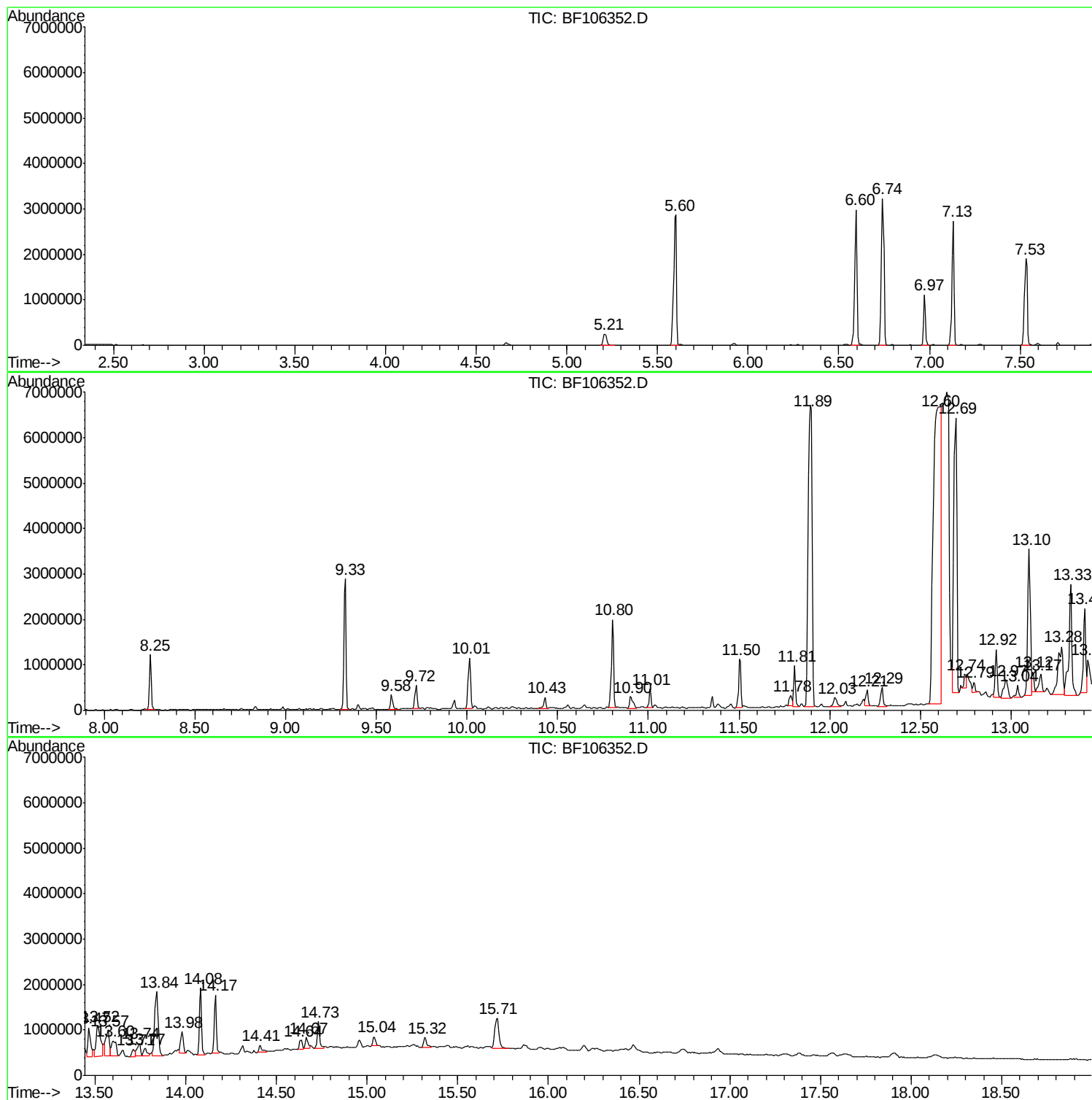
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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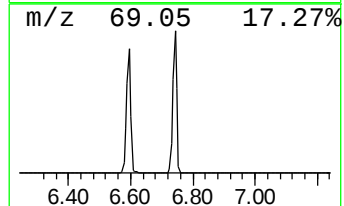
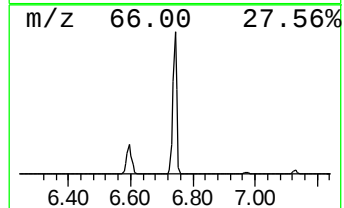
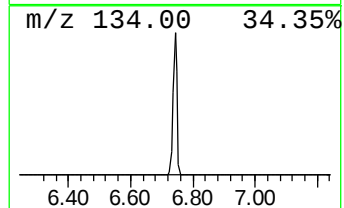
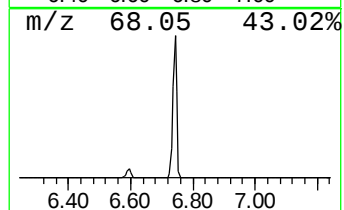
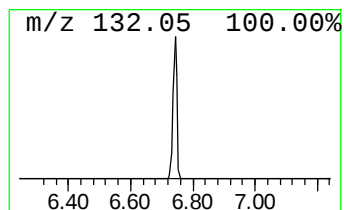
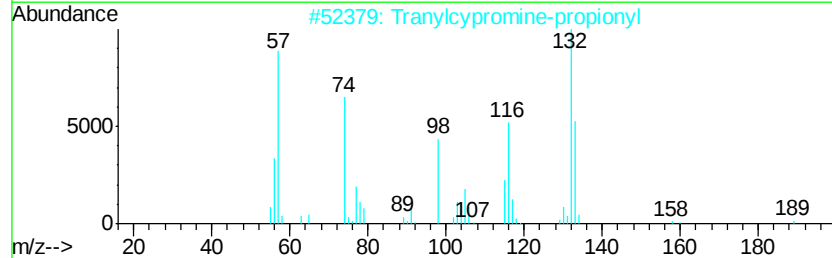
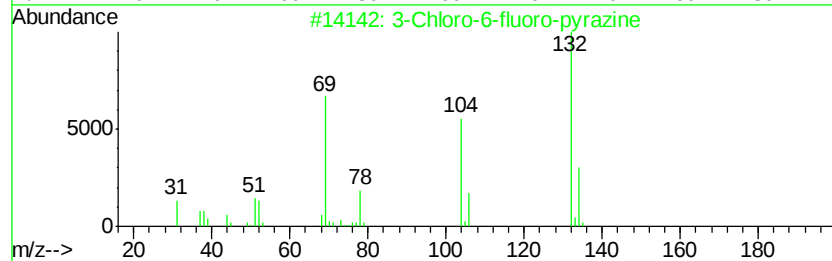
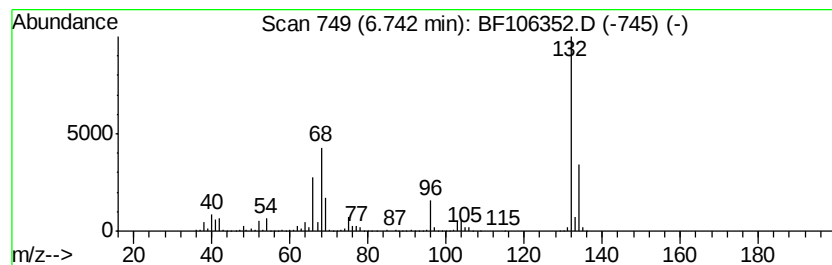
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	67.08 ng	2925200	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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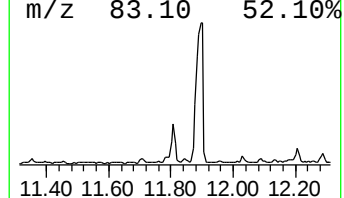
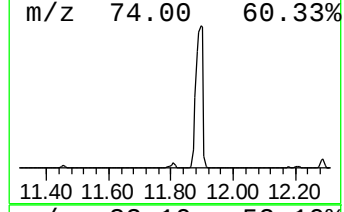
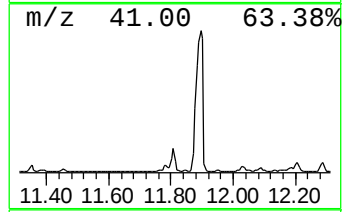
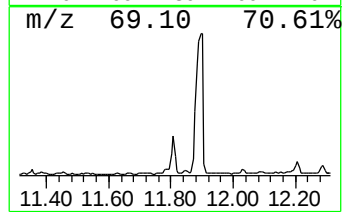
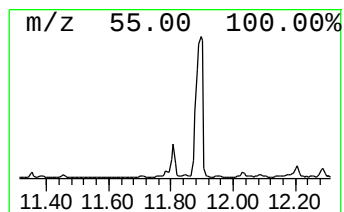
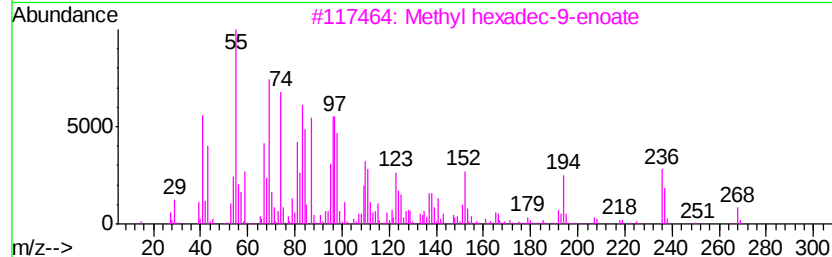
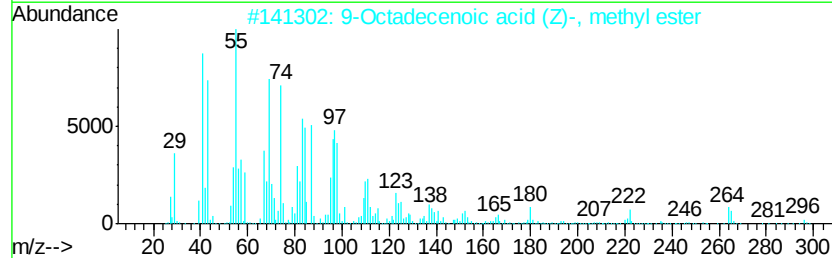
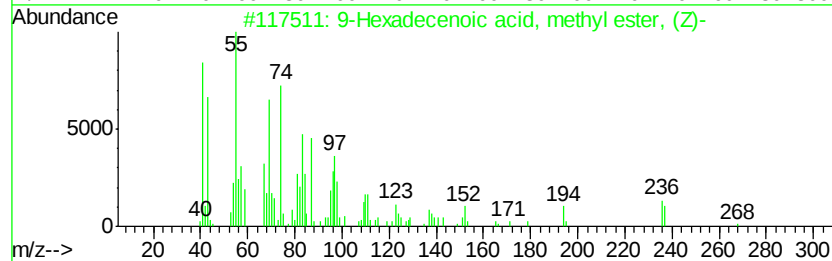
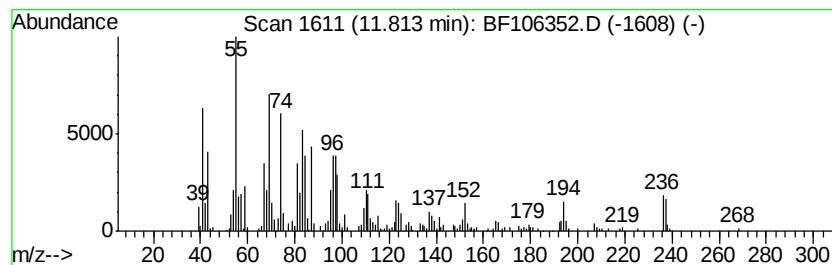
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Hexadecenoic acid, methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	13.19 ng	661106	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
3		Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	90
4		Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
5		14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	83



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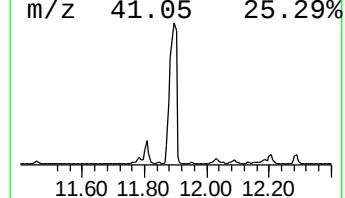
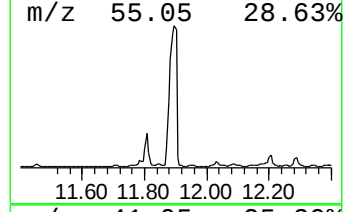
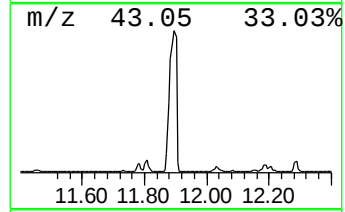
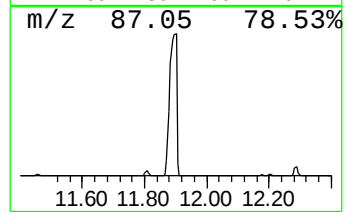
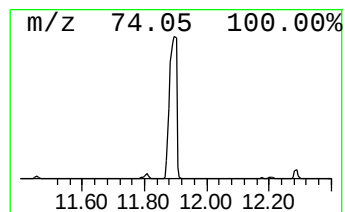
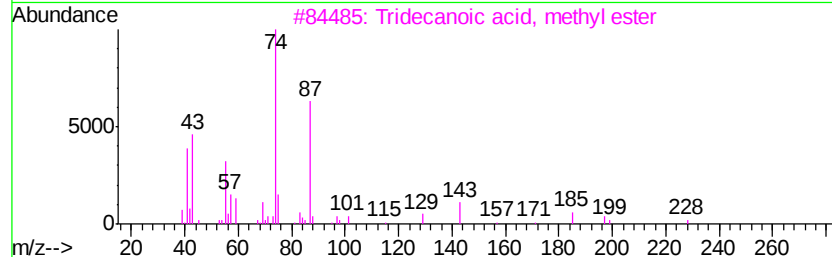
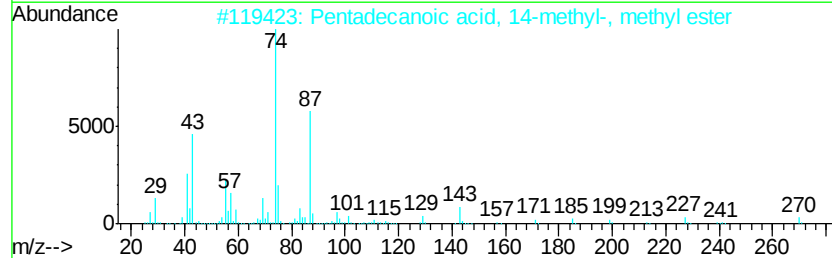
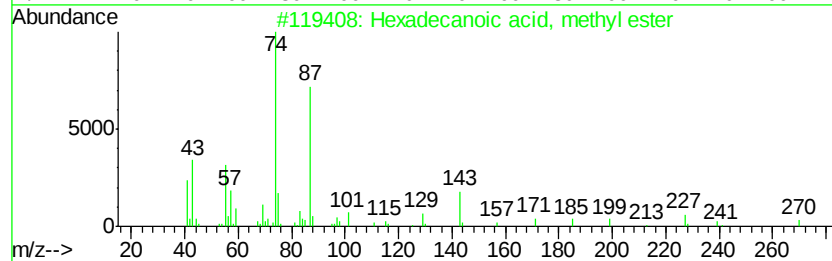
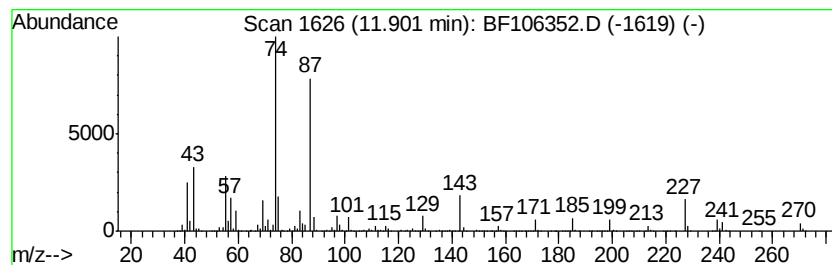
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	202.34 ng	10142100	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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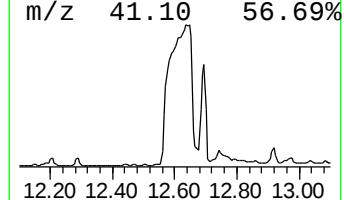
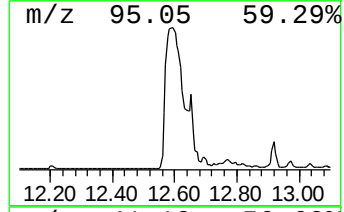
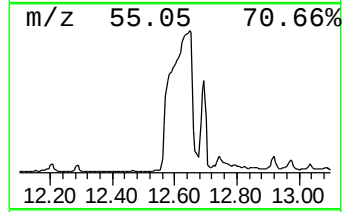
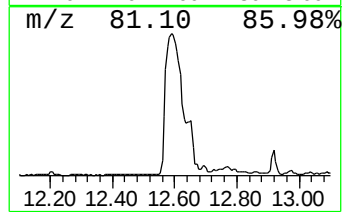
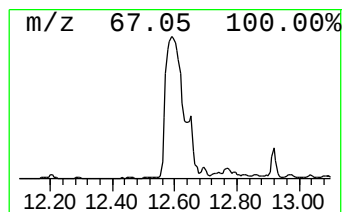
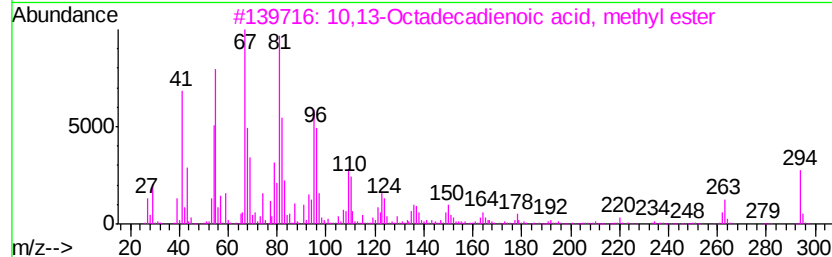
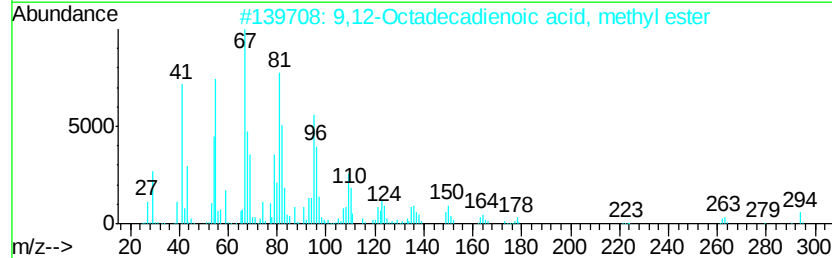
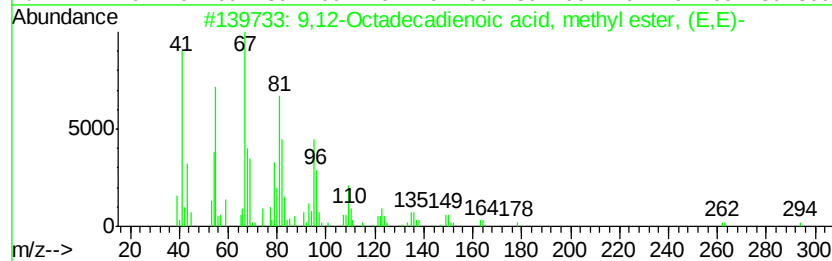
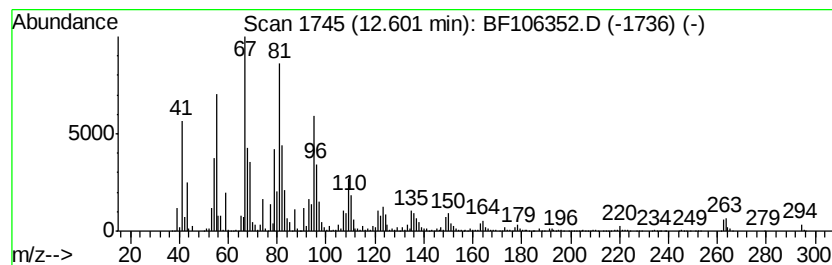
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	369.16 ng	18503700	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99



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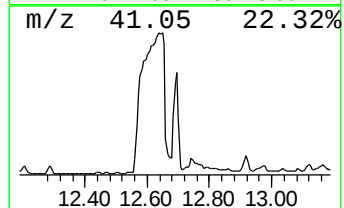
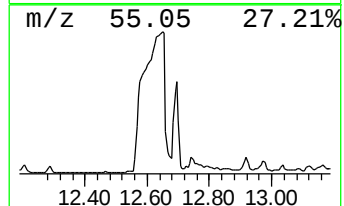
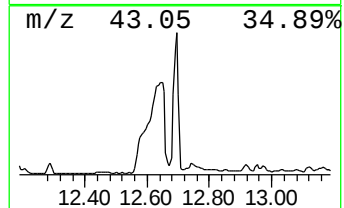
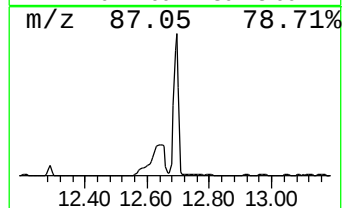
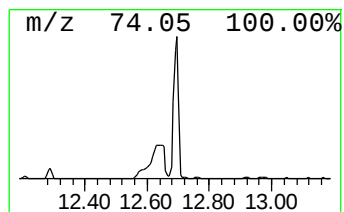
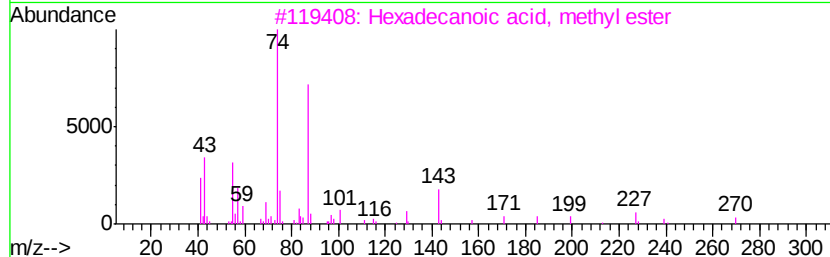
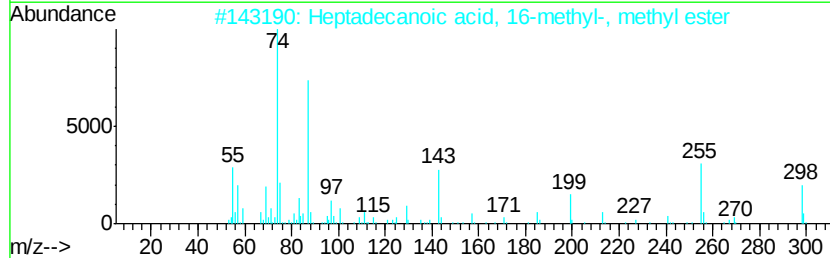
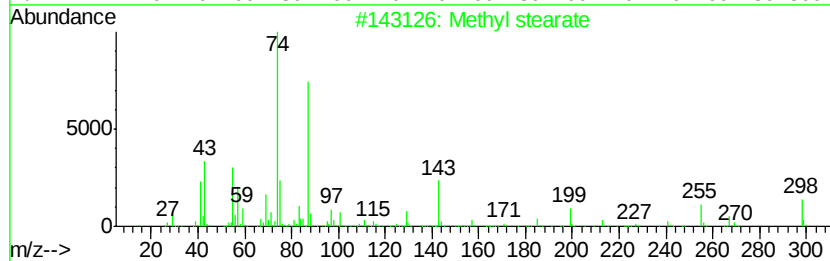
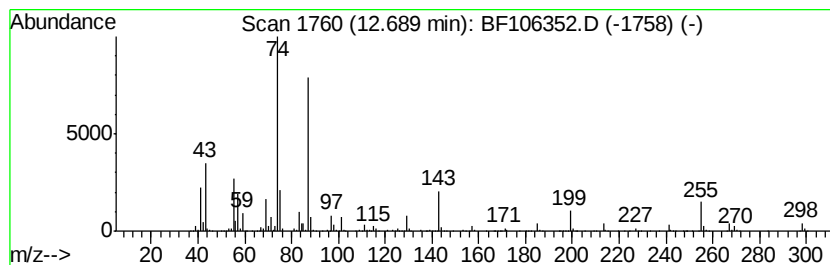
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ClientSampleId :
SB-35COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	127.08 ng	6369580	Phenanthrene-d10	11.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl stearate	298 C19H38O2	000112-61-8 98
2		Heptadecanoic acid, 16-methyl-, ...	298 C19H38O2	005129-61-3 93
3		Hexadecanoic acid, methyl ester	270 C17H34O2	000112-39-0 91
4		Heptadecanoic acid, 15-methyl-, ...	298 C19H38O2	054833-55-5 91
5		Methyl tetradecanoate	242 C15H30O2	000124-10-7 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
Acq On : 12 Jun 2018 18:43
Operator : JU/SJ
Sample : J3415-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-35COMP

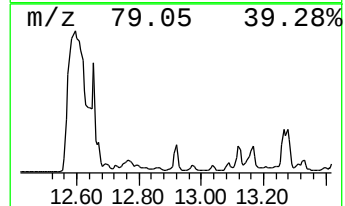
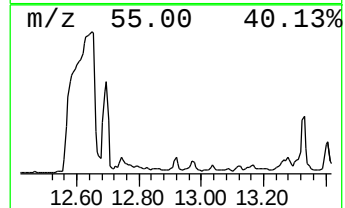
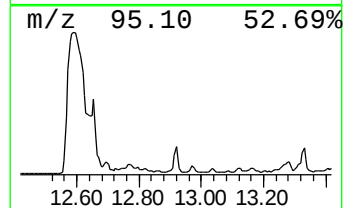
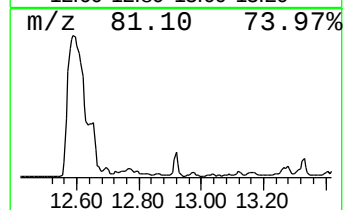
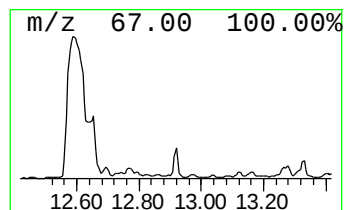
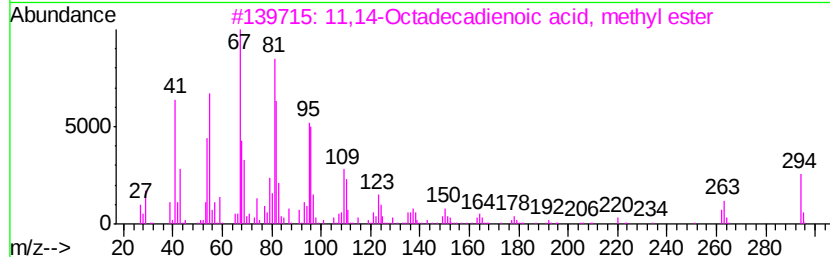
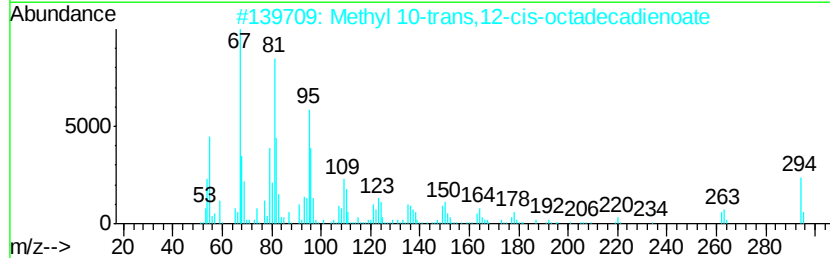
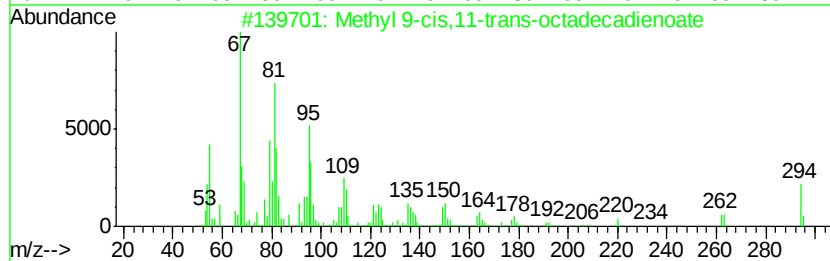
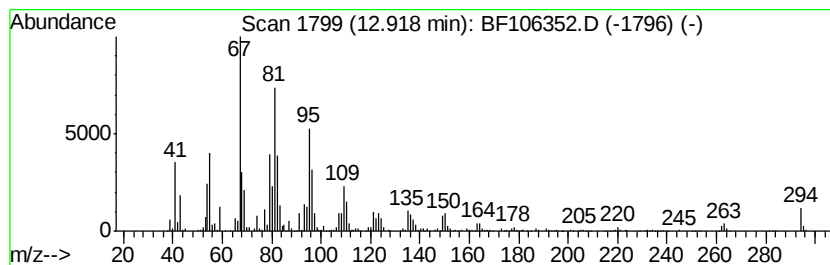
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl 9-cis,11-trans-octad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	16.88 ng	963175	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
2		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
3		11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	95
4		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5		7,10-Octadecadienoic acid, methy...	294	C19H34O2	056554-24-6	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
Acq On : 12 Jun 2018 18:43
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Sample : J3415-04
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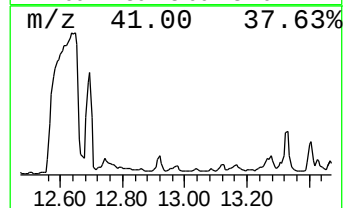
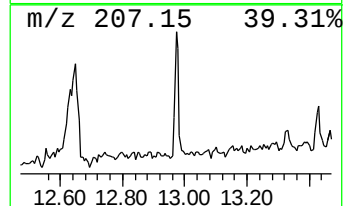
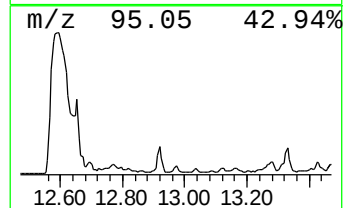
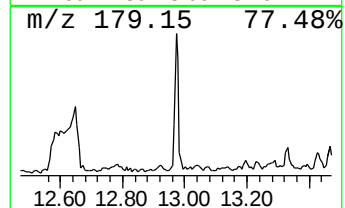
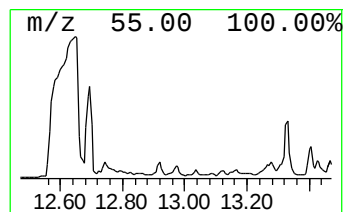
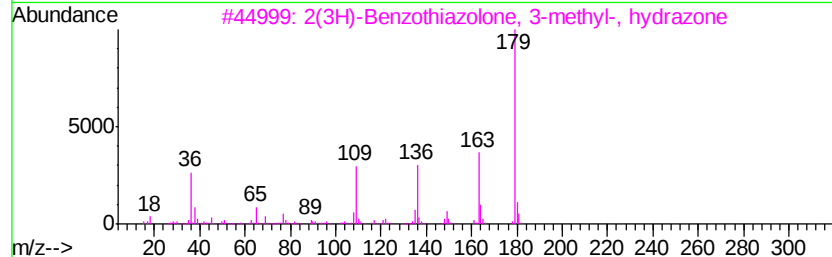
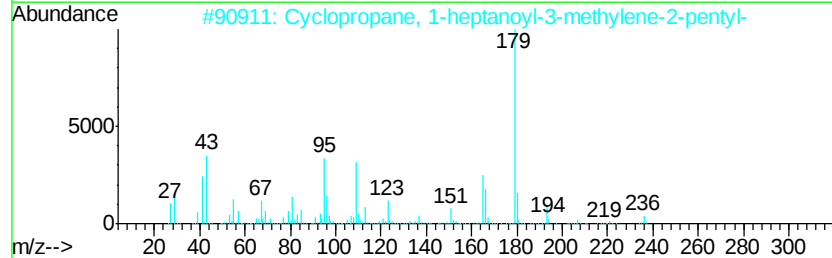
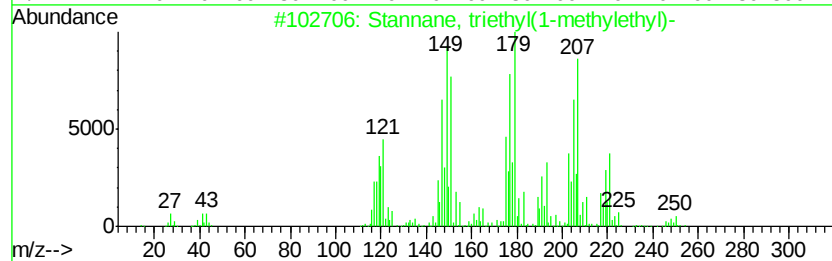
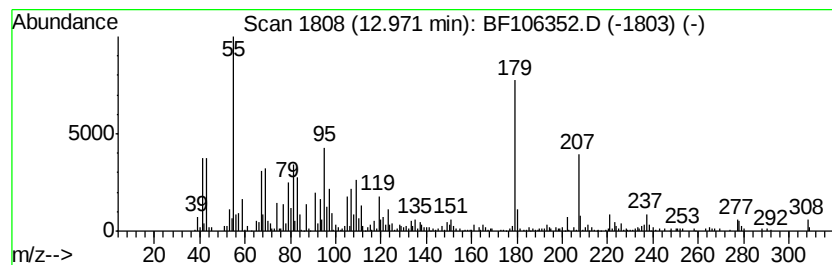
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Stannane, triethyl(1-methyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	11.19 ng	638733	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stannane, triethyl(1-methylethyl)-	250	C9H22Sn	017582-52-4	60
2		Cyclopropane, 1-heptanoyl-3-meth...	236	C16H28O	1000157-26-0	50
3		2(3H)-Benzothiazolone, 3-methyl-...	179	C8H9N3S	001128-67-2	30
4		2H-1-Benzopyran, 3,4,4a,5,6,8a-h...	194	C13H22O	041678-32-4	30
5		4,7(1H,8H)-Pteridinedione, 2-amino-	179	C6H5N5O2	000529-69-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
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Sample : J3415-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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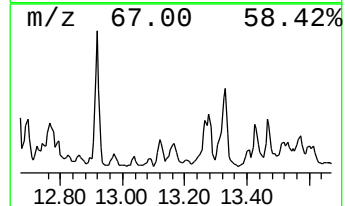
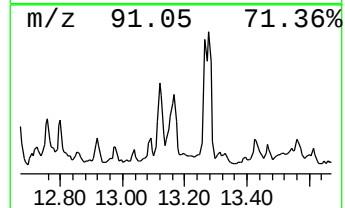
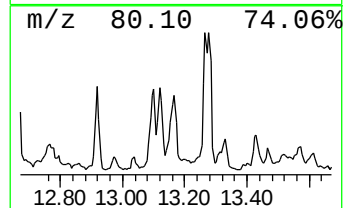
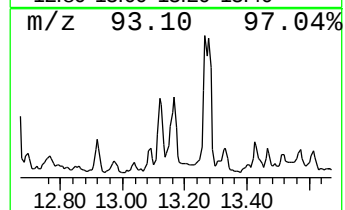
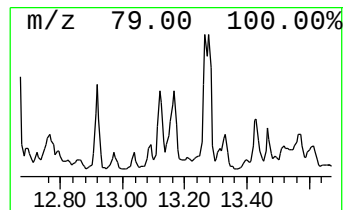
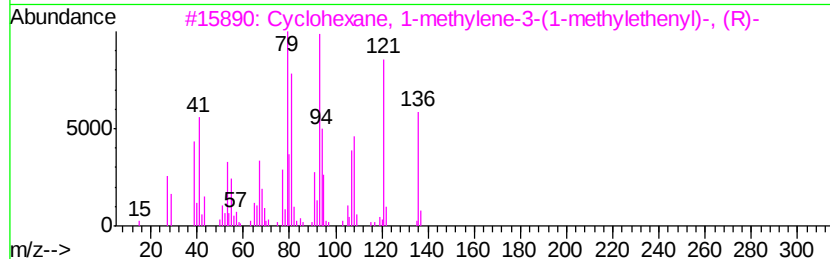
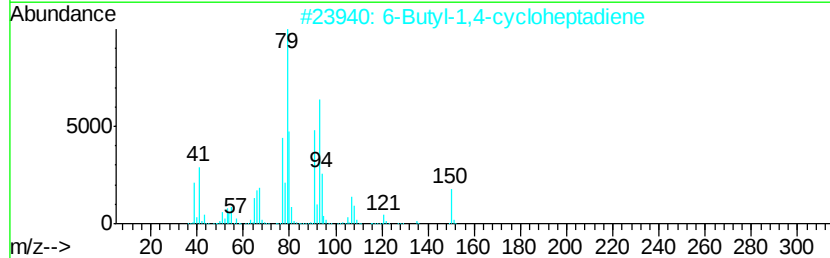
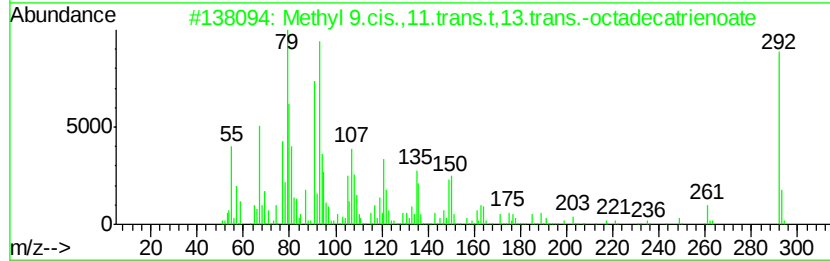
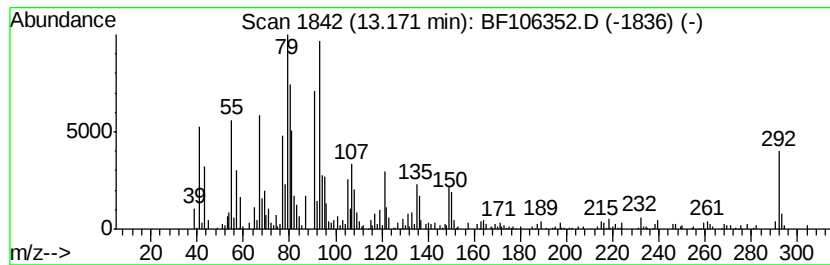
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methyl 9.cis.,11.trans.t,13... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	8.48 ng	483969	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 9.cis.,11.trans.t,13.trans...	292	C19H32O2	1000336-42-6	94
2		6-Butyl-1,4-cycloheptadiene	150	C11H18	022735-58-6	76
3		Cyclohexane, 1-methylene-3-(1-methylethenyl)-, (R)-	136	C10H16	013837-95-1	68
4		m-Mentha-4,8-diene, (1S,3S)-(+)-	136	C10H16	005208-51-5	62
5		Cyclohexene, 5-methyl-3-(1-methylethenyl)-, (R)-	136	C10H16	056816-08-1	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
Acq On : 12 Jun 2018 18:43
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Sample : J3415-04
Misc :
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ClientSampleId :
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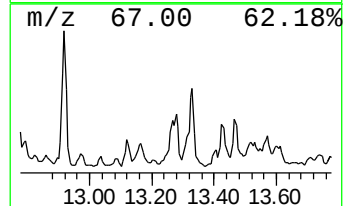
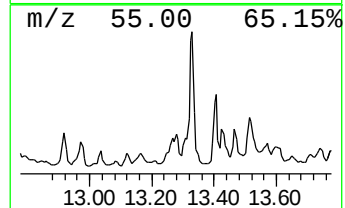
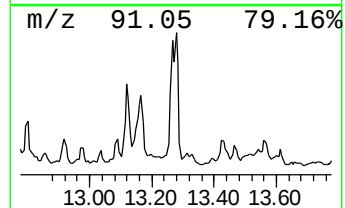
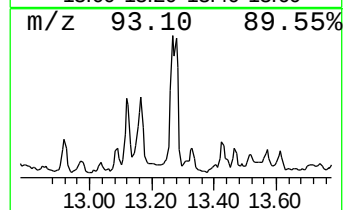
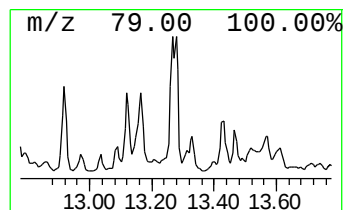
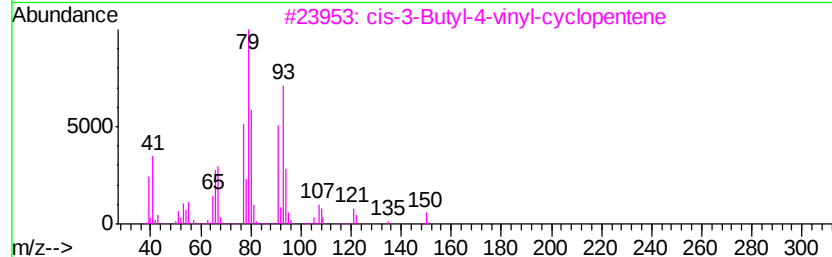
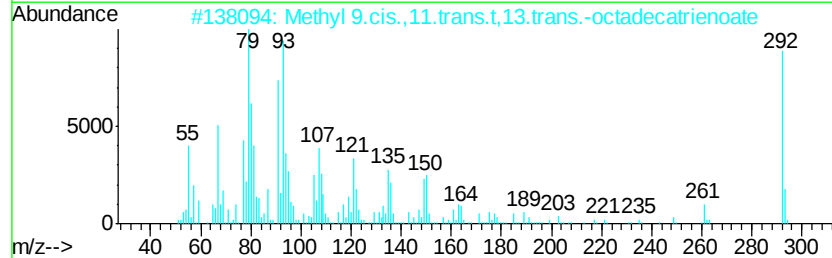
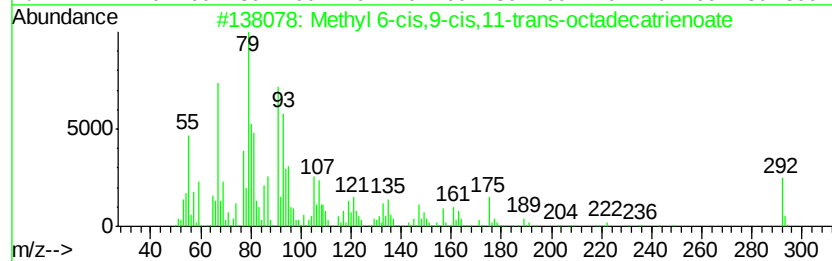
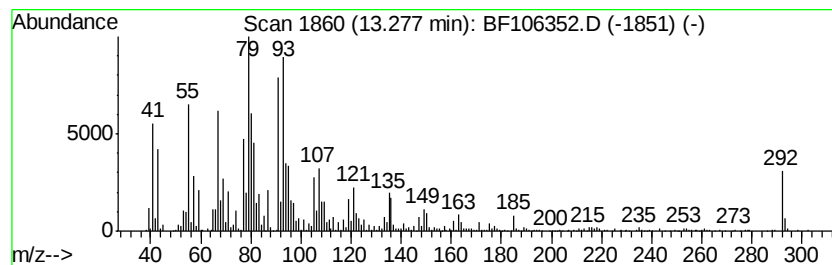
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Methyl 6-cis,9-cis,11-trans... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	33.20 ng	1894650	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1000336-37-7	90
2		Methyl 9-cis,11-trans,13-trans...	292	C19H32O2	1000336-42-6	86
3		cis-3-Butyl-4-vinyl-cyclopentene	150	C11H18	093779-52-3	76
4		3-Dodecen-1-yne, (E)-	164	C12H20	025091-25-2	72
5		Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
Acq On : 12 Jun 2018 18:43
Operator : JU/SJ
Sample : J3415-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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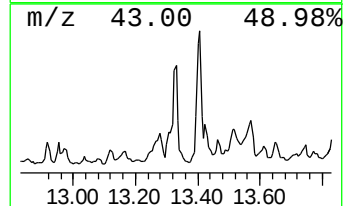
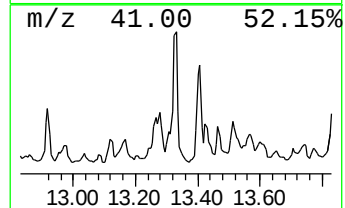
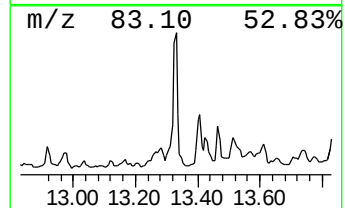
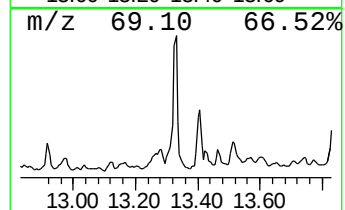
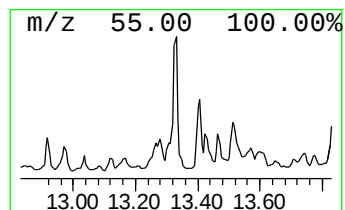
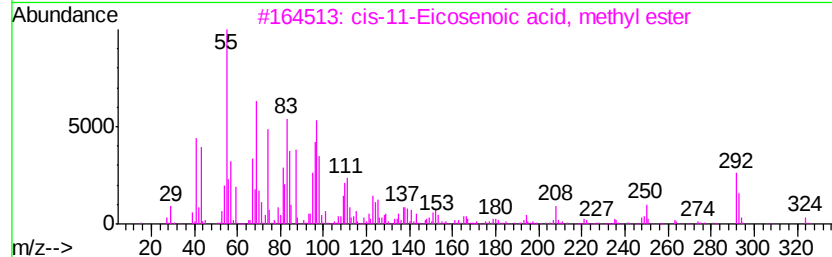
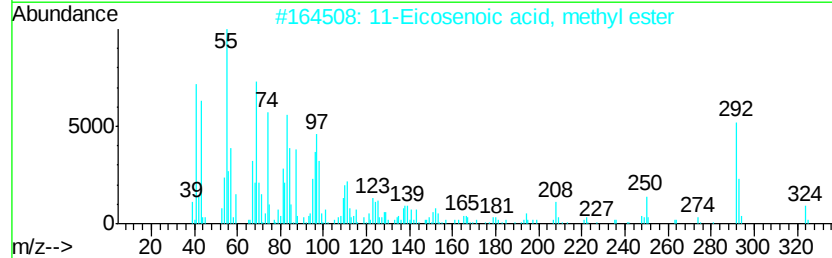
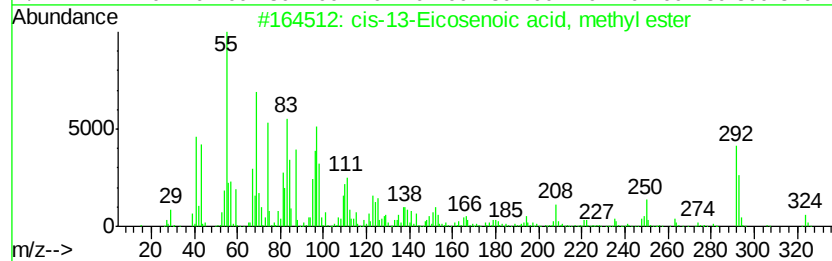
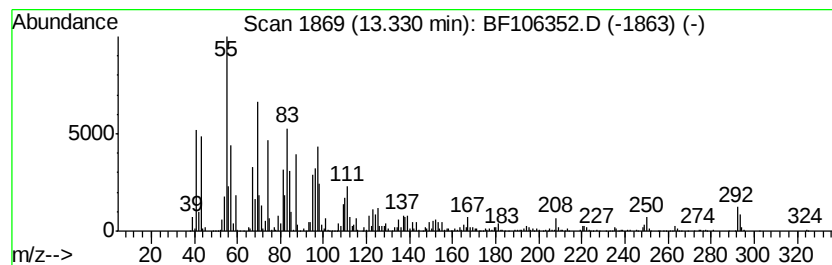
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 cis-13-Eicosenoic acid, met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	51.53 ng	2940750	Chrysene-d12	14.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	99
2			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
3			cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	91
4			Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	91
5			cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
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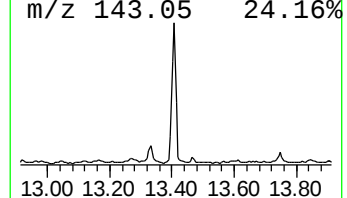
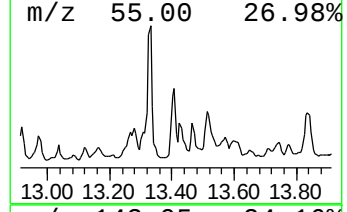
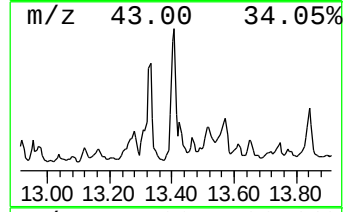
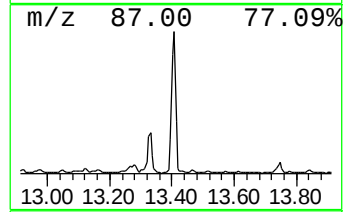
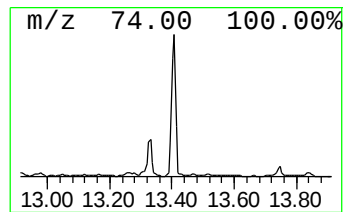
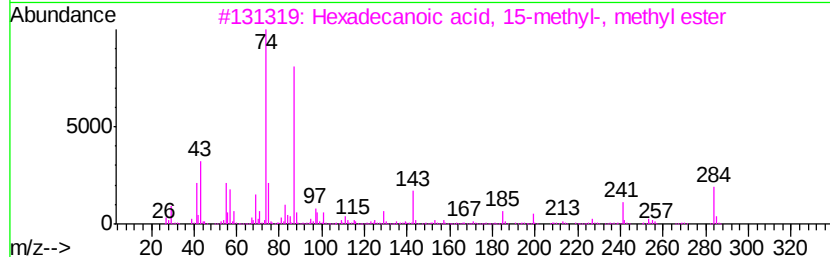
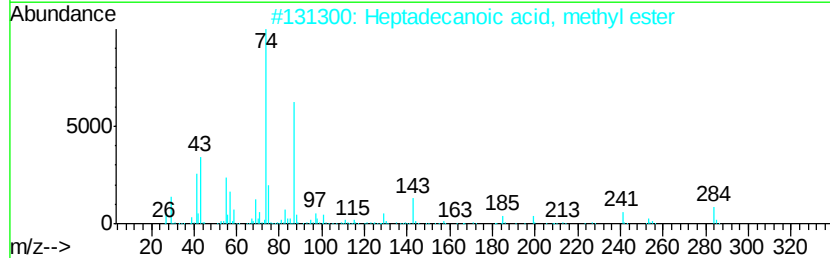
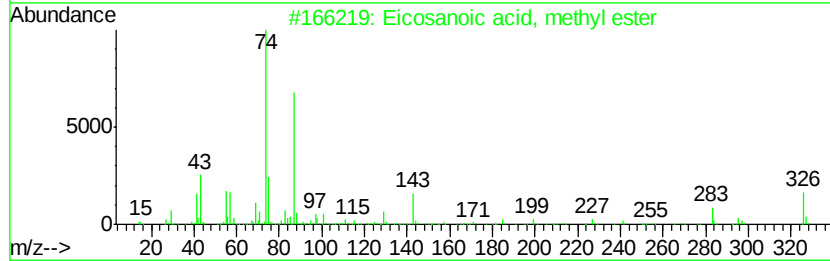
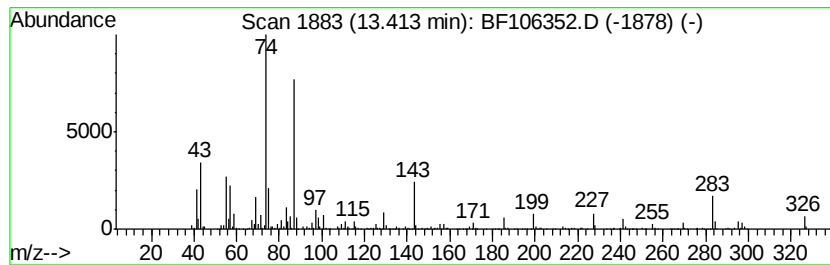
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	31.45 ng	1794590	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	95
2		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
3		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
4		Methyl stearate	298	C19H38O2	000112-61-8	91
5		Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106352.D
Acq On : 12 Jun 2018 18:43
Operator : JU/SJ
Sample : J3415-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-35COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 E,E-6,11-Tridecadien-1-ol a... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	12.44 ng	709960	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E,E-6,11-Tridecadien-1-ol acetate	238	C15H26O2	1000130-97-2	52
2		Methyl 10,11-octadecadienoate	294	C19H34O2	1000336-45-3	44
3		exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	154	C10H18O	1000374-19-3	43
4		1,E-8,Z-10-Tridecatriene	178	C13H22	080625-30-5	40
5		Perhydrophenalene, (3a.alpha., 6...	178	C13H22	040250-64-4	38

