

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
 Data File : BF112760.D
 Acq On : 28 Feb 2019 14:15
 Operator : JU/SJ
 Sample : K1340-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-022719

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-BF022719.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	5.351	550	555	559	rBV	3821070	4076056	93.87%	8.978%
2	6.028	667	670	674	rBV	128764	119026	2.74%	0.262%
3	6.381	724	730	733	rBV	4169984	4342107	100.00%	9.564%
4	6.516	748	753	756	rBV	4347218	4289987	98.80%	9.449%
5	6.745	788	792	795	rBV	1537018	1226387	28.24%	2.701%
6	6.904	815	819	822	rBV	3397446	3204188	73.79%	7.058%
7	7.304	882	887	890	rBV	2921001	2641960	60.85%	5.819%
8	8.028	1006	1010	1013	rBV	1692147	1508371	34.74%	3.322%
9	9.098	1188	1192	1196	rBV	4438265	4234480	97.52%	9.327%
10	9.439	1248	1250	1254	rVB	268902	228805	5.27%	0.504%
11	9.492	1255	1259	1262	rBV	415998	345483	7.96%	0.761%
12	9.633	1279	1283	1286	rBV	85760	73064	1.68%	0.161%
13	9.774	1303	1307	1311	rBV	1913801	1618731	37.28%	3.565%
14	10.292	1389	1395	1398	rBV4	150739	151278	3.48%	0.333%
15	10.557	1436	1440	1443	rBV	3178262	2787926	64.21%	6.141%
16	10.780	1474	1478	1481	rBV3	40804	46831	1.08%	0.103%
17	10.927	1499	1503	1505	rBV	63250	54065	1.25%	0.119%
18	11.139	1533	1539	1542	rBV5	33259	50195	1.16%	0.111%
19	11.221	1548	1553	1555	rBV2	63920	76813	1.77%	0.169%
20	11.251	1555	1558	1561	rVV	1959022	1665291	38.35%	3.668%
21	11.274	1561	1562	1565	rVV	111105	60100	1.38%	0.132%
22	11.321	1565	1570	1573	rVB4	56638	91608	2.11%	0.202%
23	11.486	1595	1598	1604	rVB3	41552	44084	1.02%	0.097%
24	11.657	1624	1627	1632	rVB	147677	129756	2.99%	0.286%
25	11.727	1632	1639	1641	rBV2	58693	115229	2.65%	0.254%
26	11.792	1645	1650	1654	rBV	773007	750222	17.28%	1.652%
27	12.063	1694	1696	1699	rVB	63840	52409	1.21%	0.115%
28	12.298	1733	1736	1740	rBV	158195	147465	3.40%	0.325%
29	12.339	1740	1743	1745	rBV	403971	369607	8.51%	0.814%
30	12.363	1745	1747	1749	rVB	421755	327320	7.54%	0.721%
31	12.457	1759	1763	1765	rBV2	215977	230111	5.30%	0.507%
32	12.510	1769	1772	1777	rVB	141576	151973	3.50%	0.335%
33	12.574	1779	1783	1787	rBV	243402	267090	6.15%	0.588%
34	12.680	1797	1801	1804	rBV	188144	217480	5.01%	0.479%

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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

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35	12.833	1823	1827	1831	rBV	4125051	3827902	88.16%	8.431%
36	13.080	1867	1869	1872	rVB	87219	68742	1.58%	0.151%
37	13.262	1898	1900	1902	rBV	52417	49810	1.15%	0.110%
38	13.739	1977	1981	1987	rBV3	353900	476445	10.97%	1.049%
39	13.874	2000	2004	2007	rBV	1529697	1527728	35.18%	3.365%
40	14.062	2033	2036	2039	rBV	159586	155255	3.58%	0.342%
41	14.368	2085	2088	2093	rBV	361129	351064	8.09%	0.773%
42	14.662	2136	2138	2145	rVB	231516	258120	5.94%	0.569%
43	14.733	2148	2150	2154	rVB	261621	237246	5.46%	0.523%
44	14.986	2190	2193	2202	rVB3	313741	465503	10.72%	1.025%
45	15.292	2241	2245	2248	rVB	901950	1009564	23.25%	2.224%
46	16.627	2467	2472	2479	rVB3	718336	1277701	29.43%	2.814%

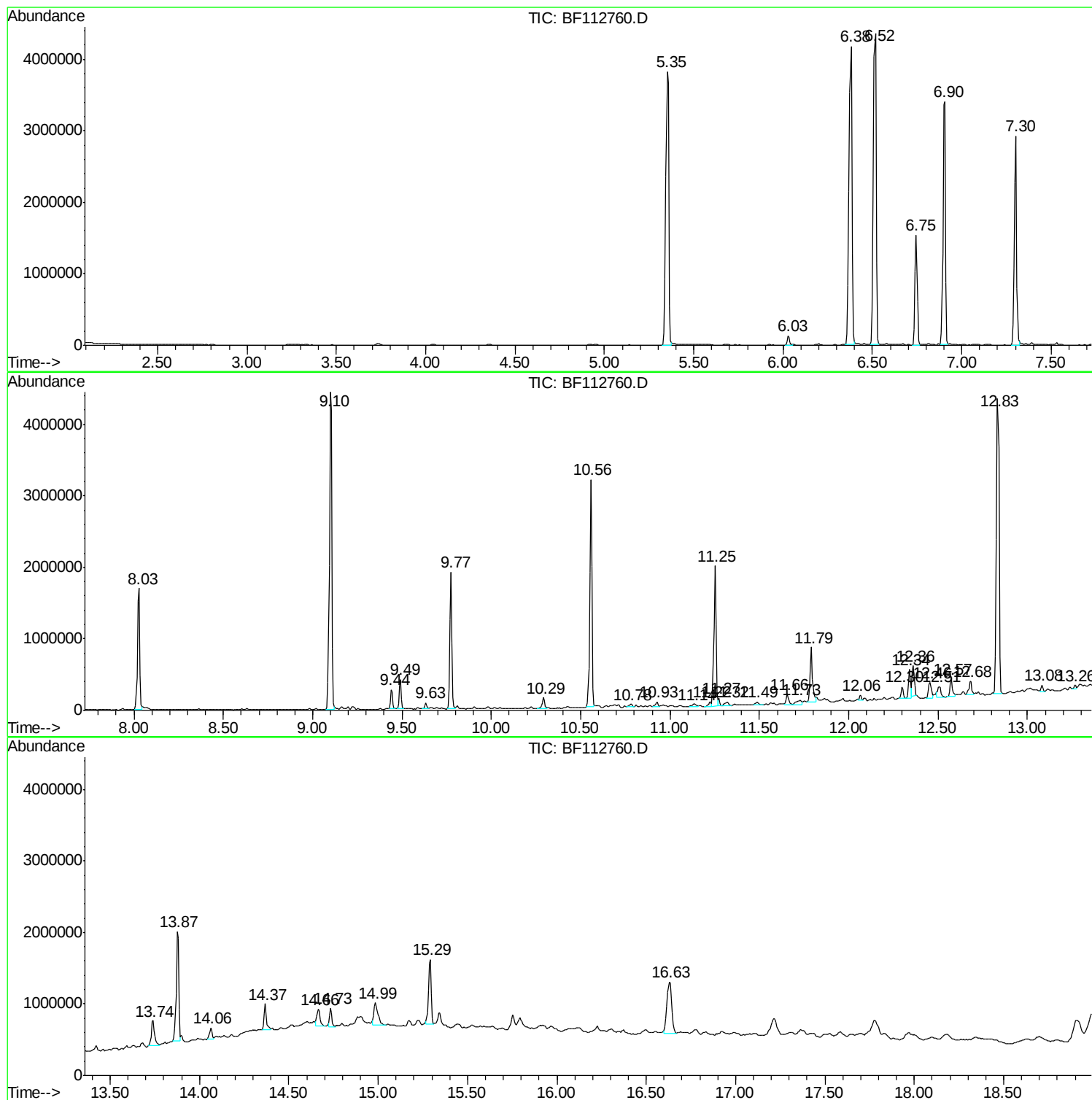
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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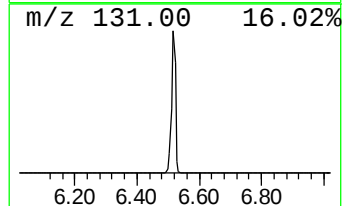
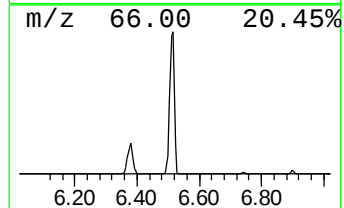
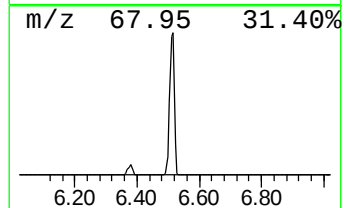
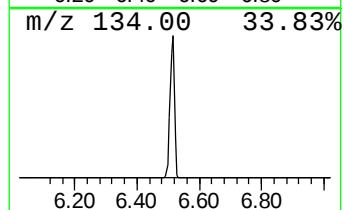
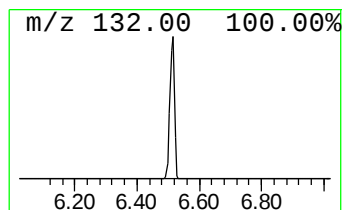
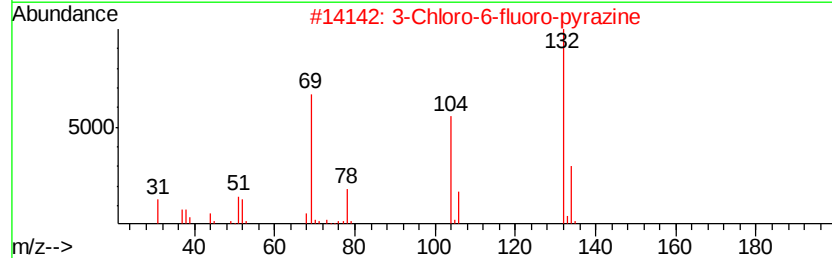
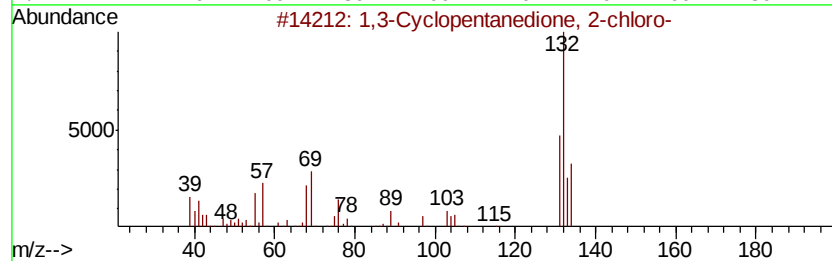
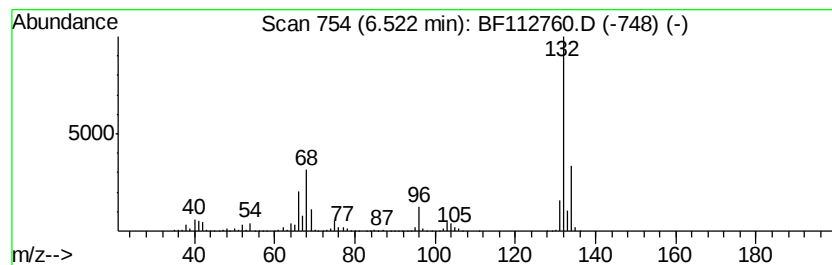
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	69.96 ng	4289990	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	47
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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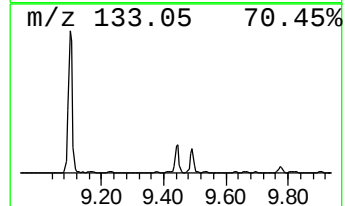
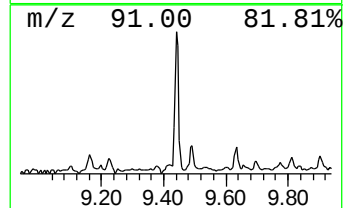
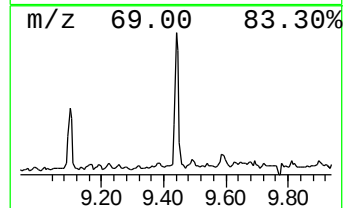
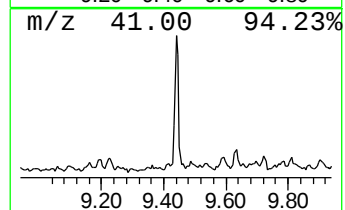
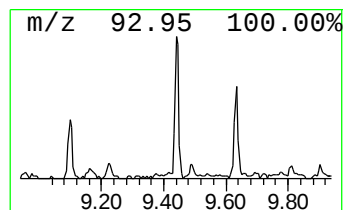
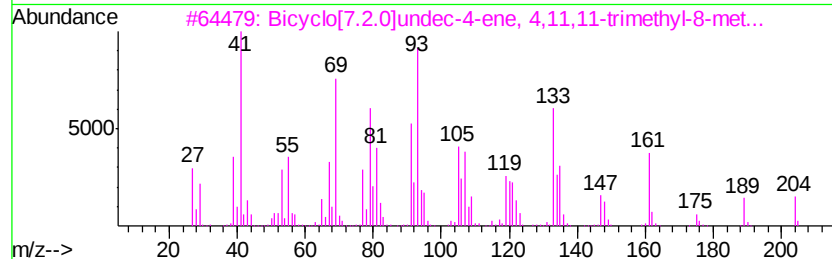
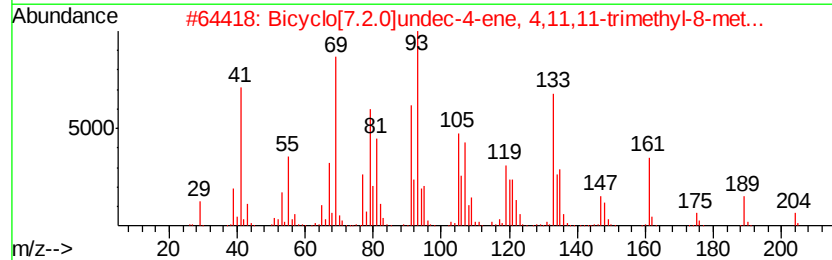
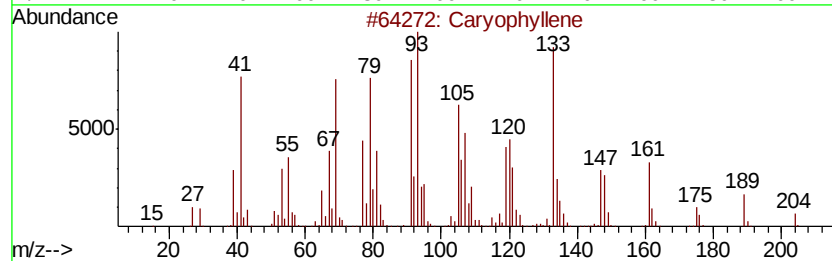
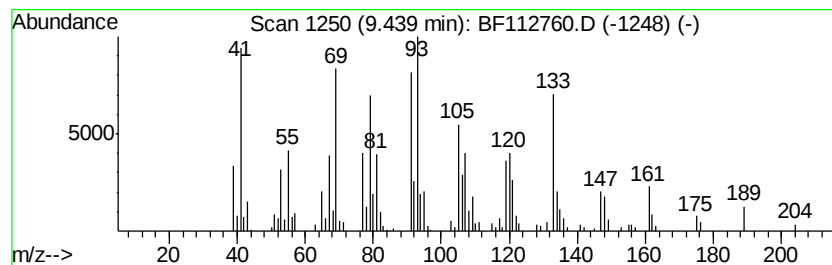
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Caryophyllene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	2.83 ng	228805	Acenaphthene-d10	9.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carvophyllene	204	C15H24	000087-44-5	99
2		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	94
3		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	93
4		Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	92
5		.alpha.-Farnesene	204	C15H24	000502-61-4	49



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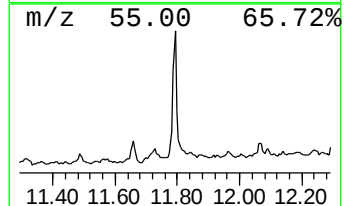
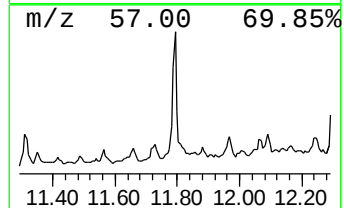
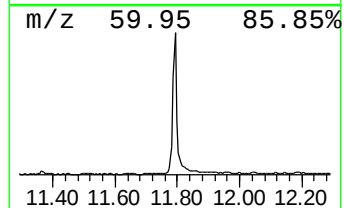
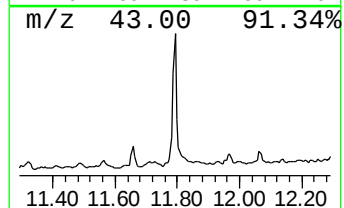
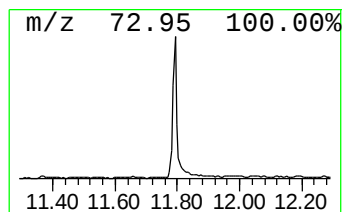
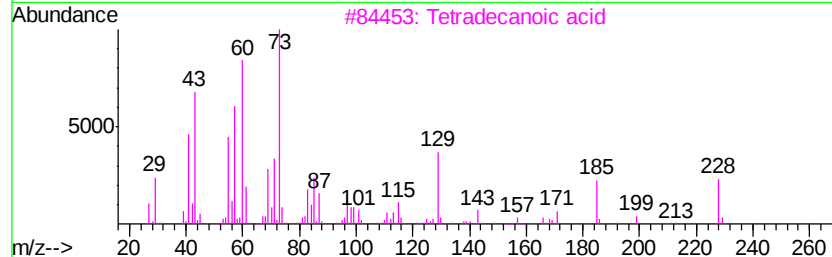
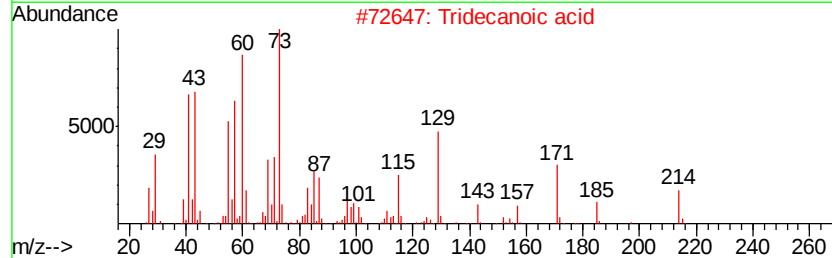
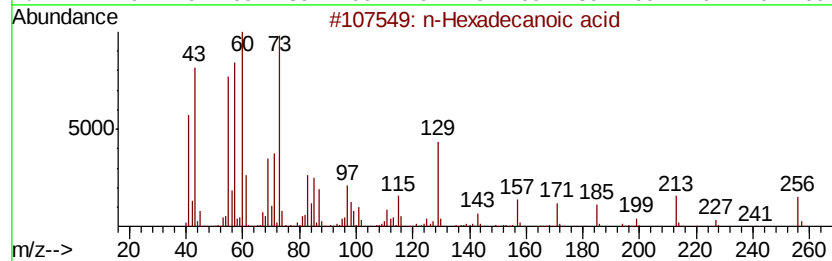
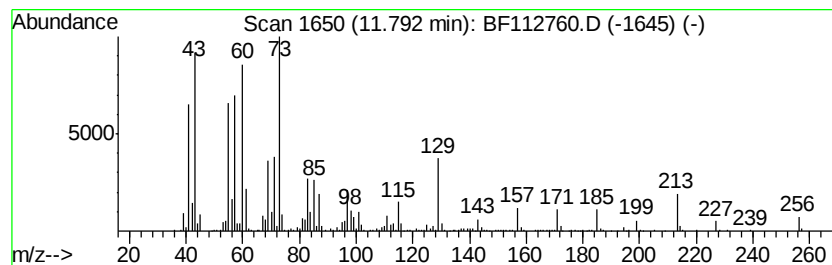
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	9.01 ng	750222	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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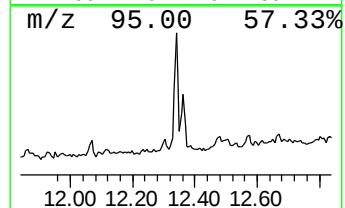
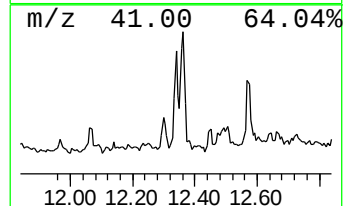
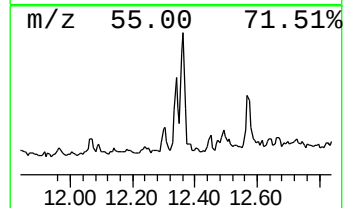
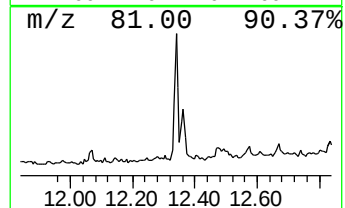
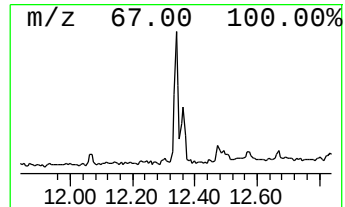
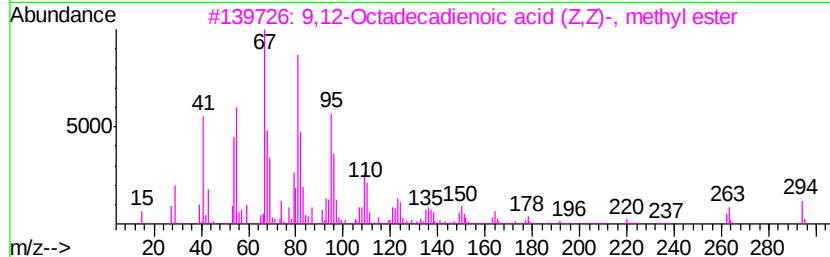
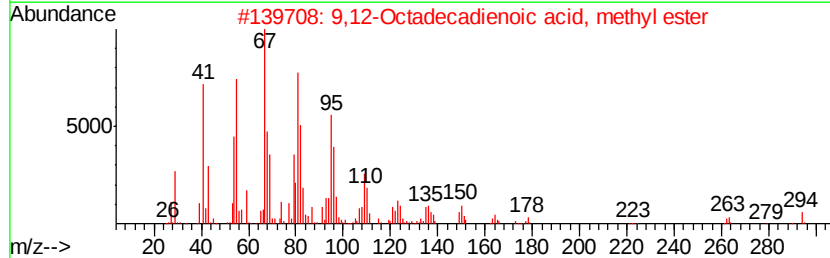
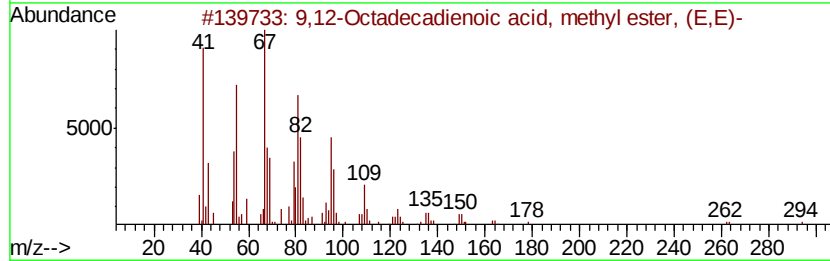
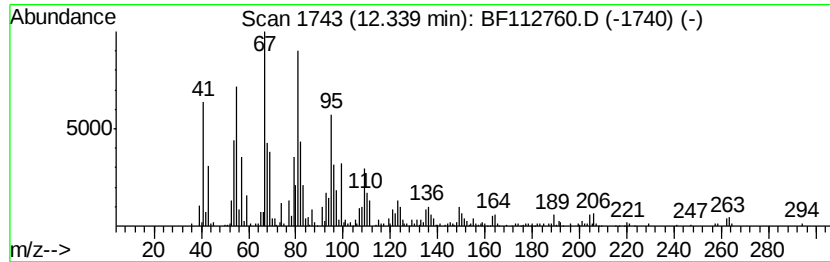
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.34	4.44 ng	369607	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	97
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	96
4	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	95
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93



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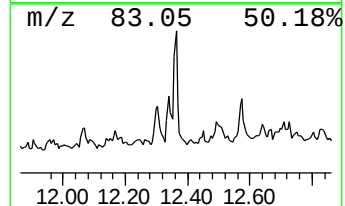
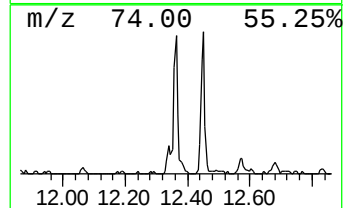
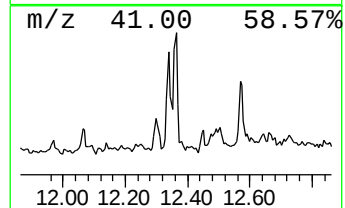
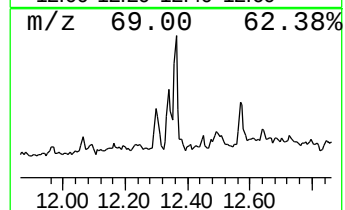
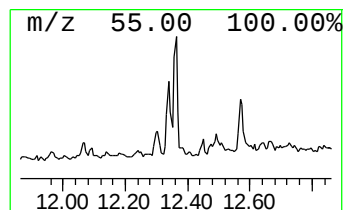
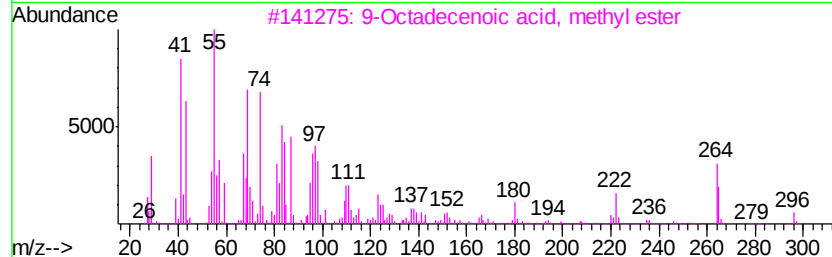
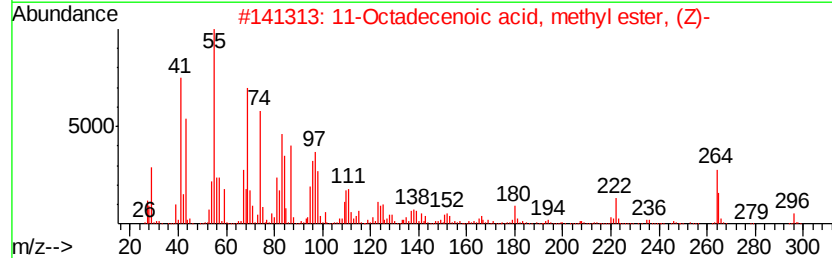
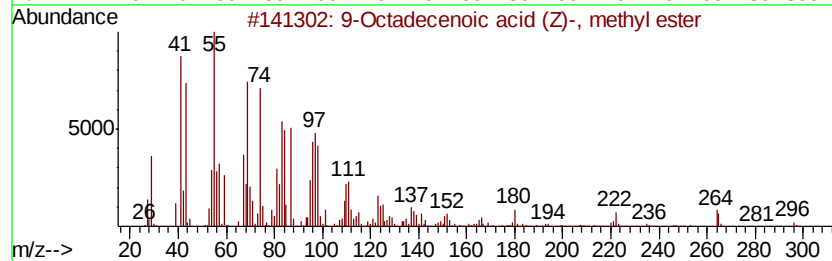
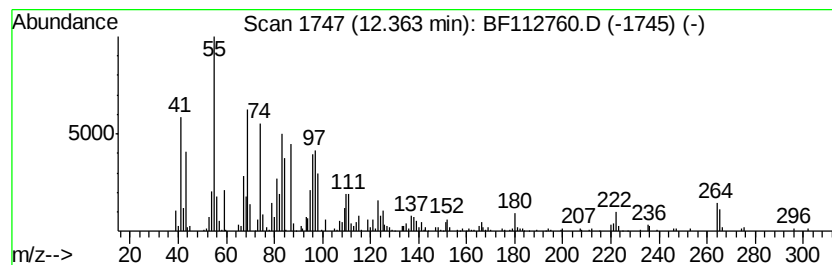
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.36	3.93 ng	327320	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112760.D
Acq On : 28 Feb 2019 14:15
Operator : JU/SJ
Sample : K1340-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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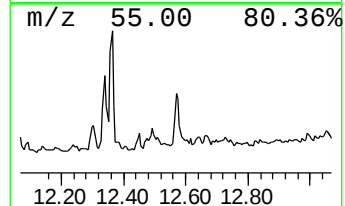
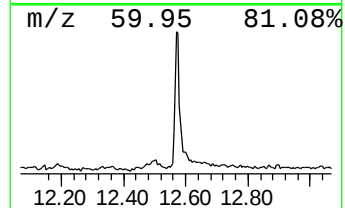
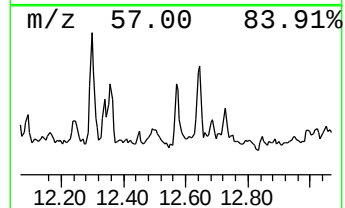
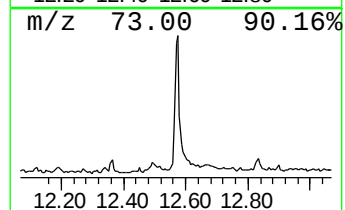
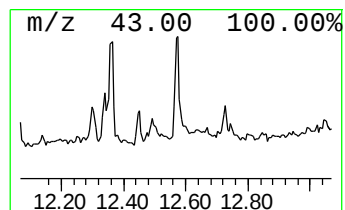
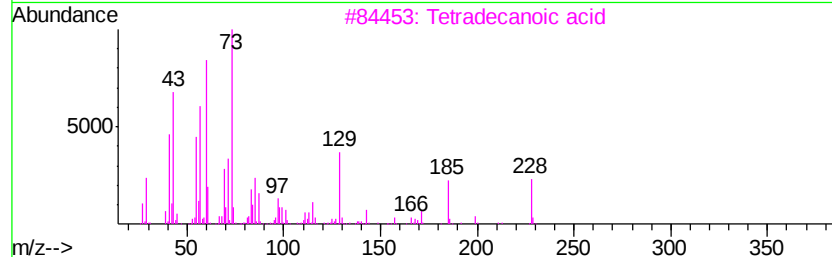
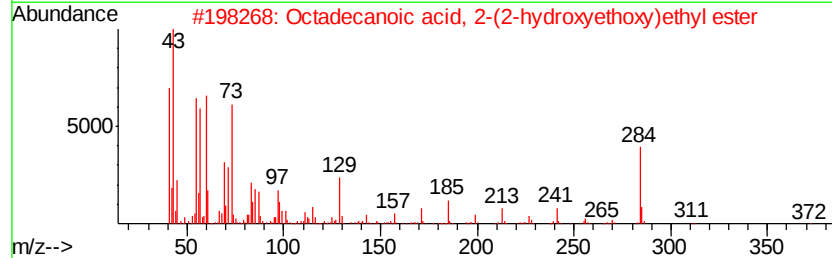
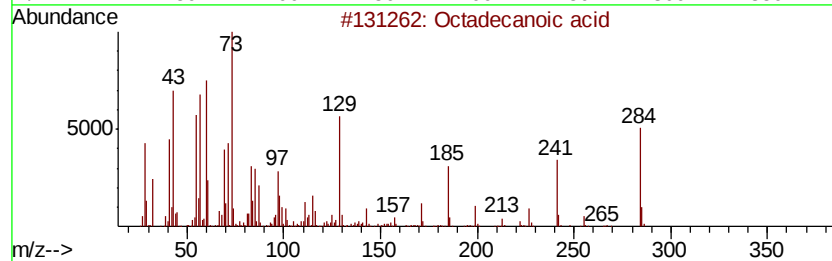
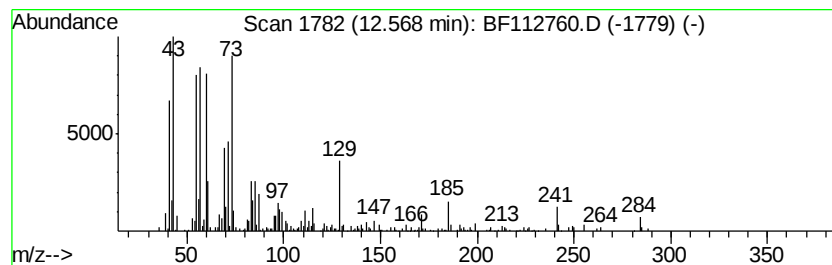
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.50 ng	267090	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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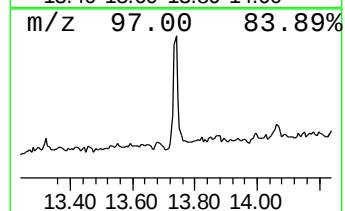
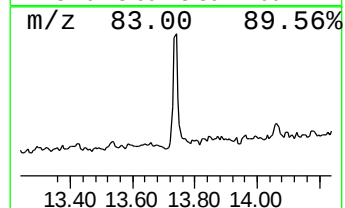
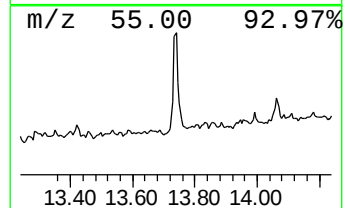
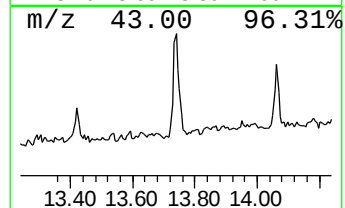
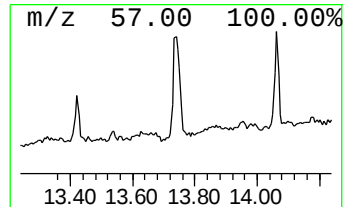
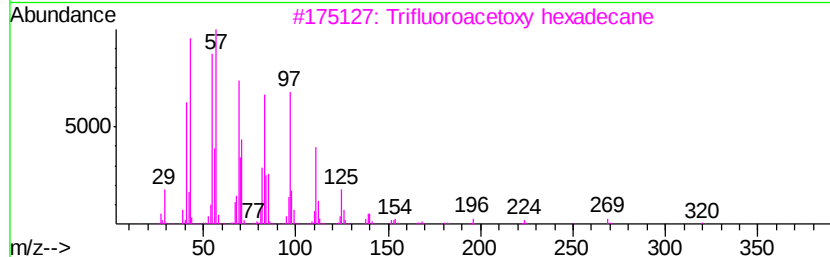
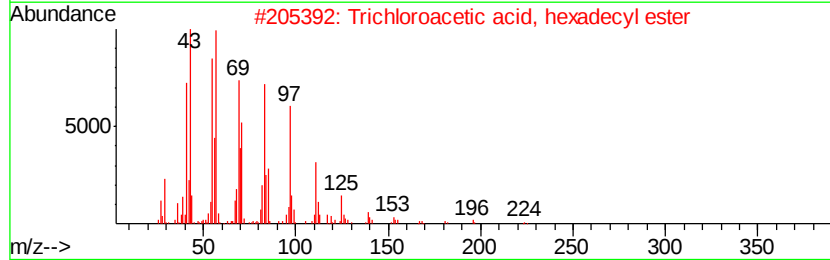
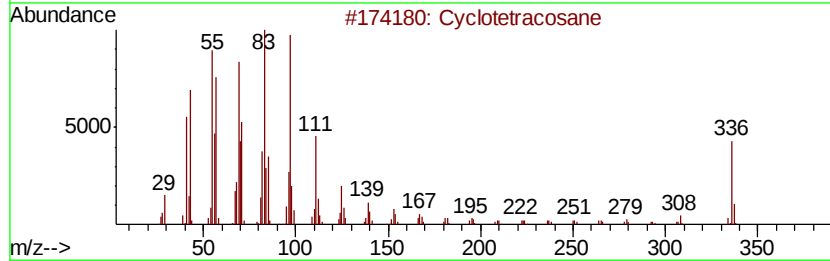
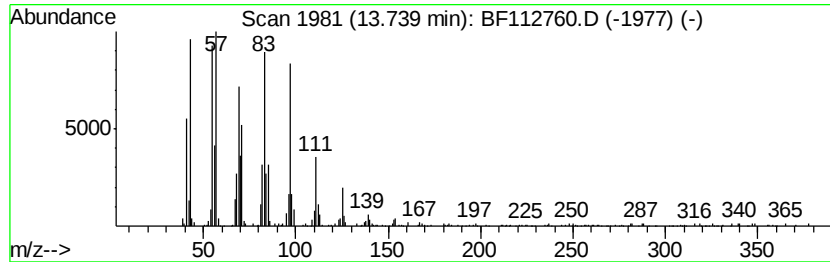
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	6.24 ng	476445	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	98
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112760.D
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Sample : K1340-01
Misc :
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ClientSampleId :
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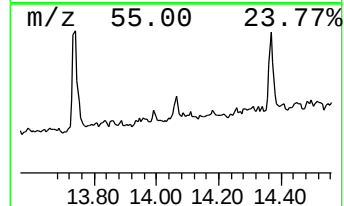
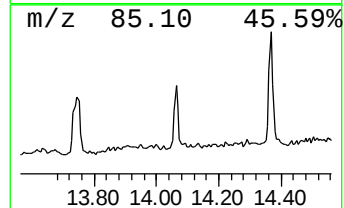
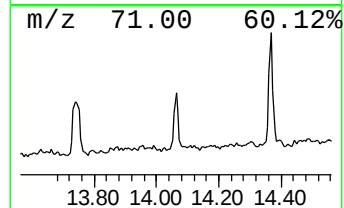
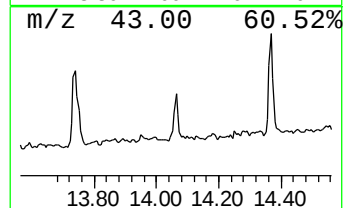
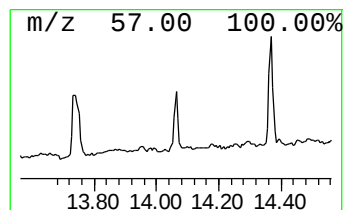
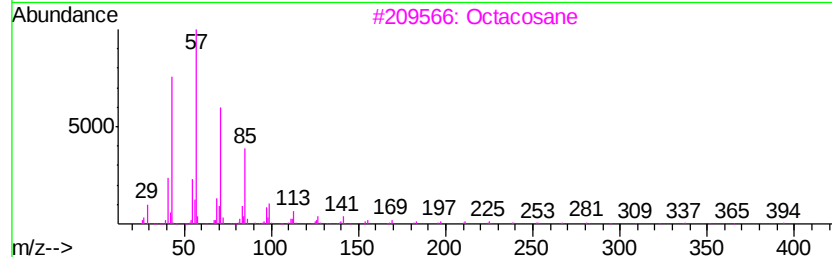
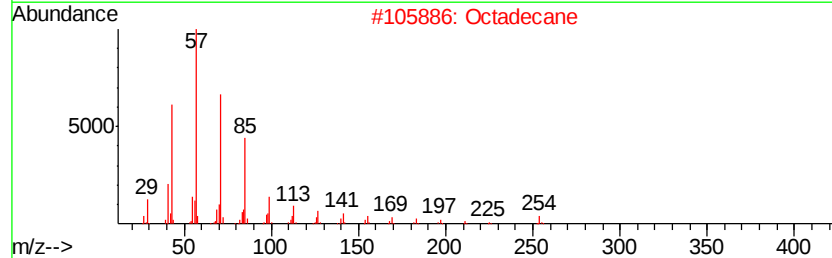
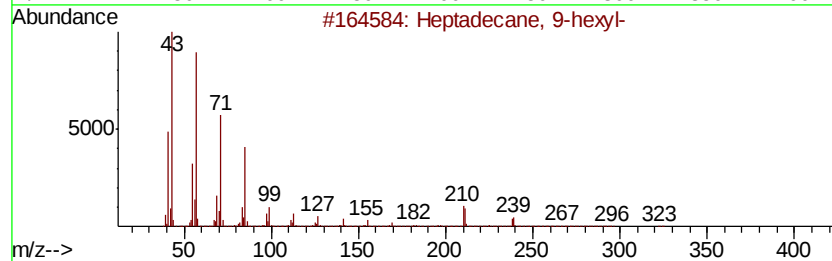
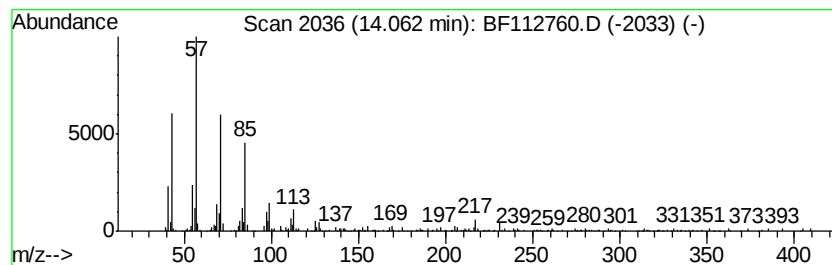
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-hexyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.03 ng	155255	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
2		Octadecane	254	C18H38	000593-45-3	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Docosane	310	C22H46	000629-97-0	87
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112760.D
Acq On : 28 Feb 2019 14:15
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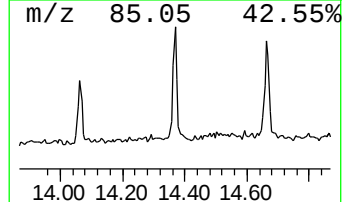
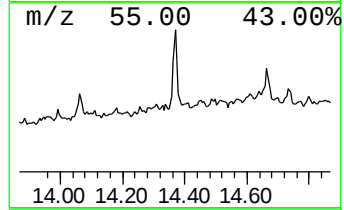
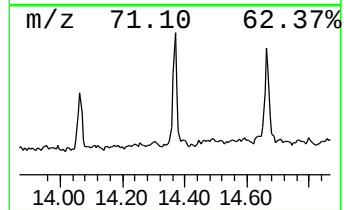
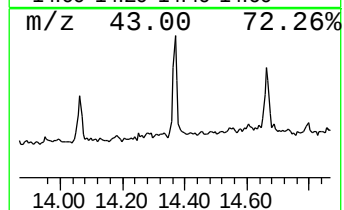
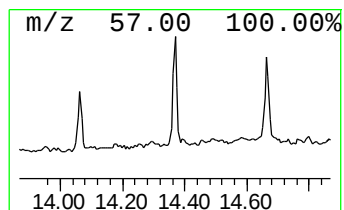
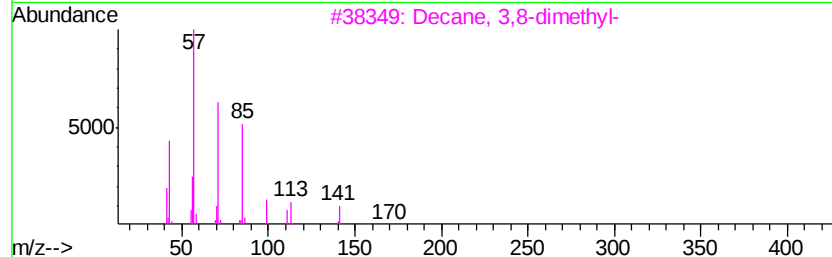
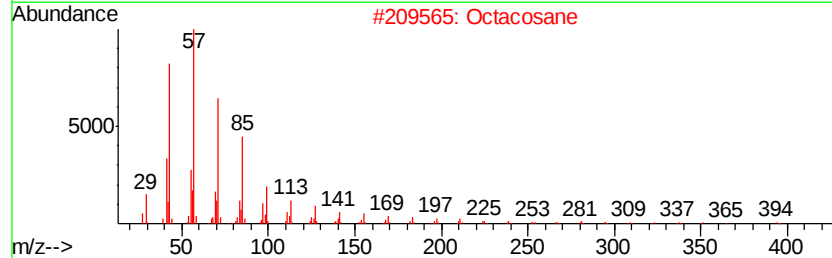
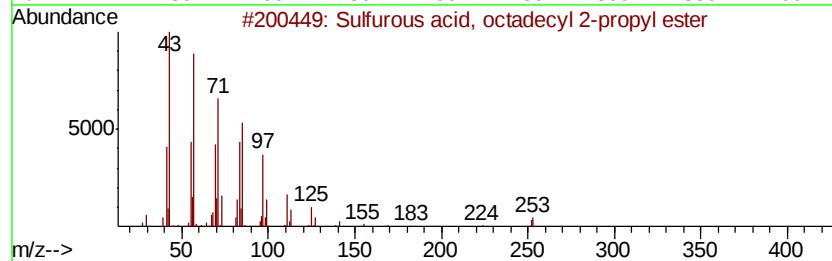
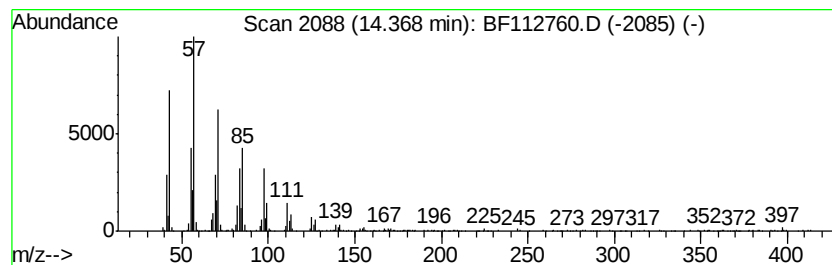
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Sulfurous acid, octadecyl 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	4.60 ng	351064	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2		Octacosane	394	C28H58	000630-02-4	70
3		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	70
4		Hexadecane	226	C16H34	000544-76-3	68
5		Pentadecane	212	C15H32	000629-62-9	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112760.D
Acq On : 28 Feb 2019 14:15
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ClientSampleId :
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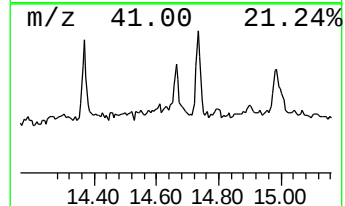
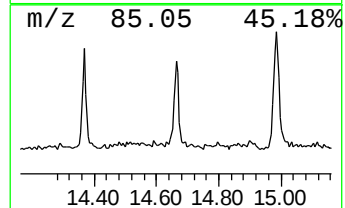
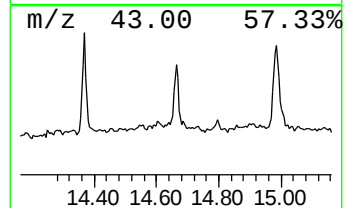
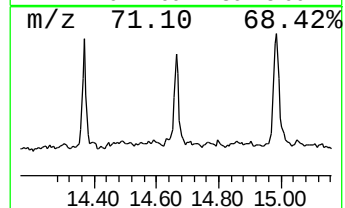
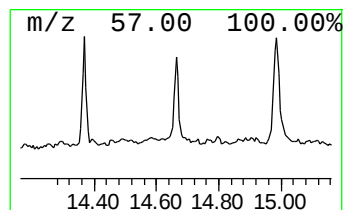
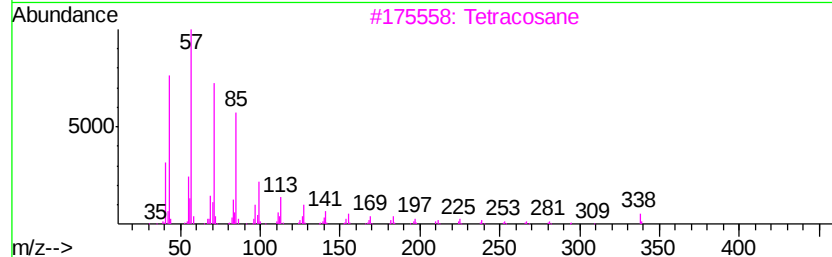
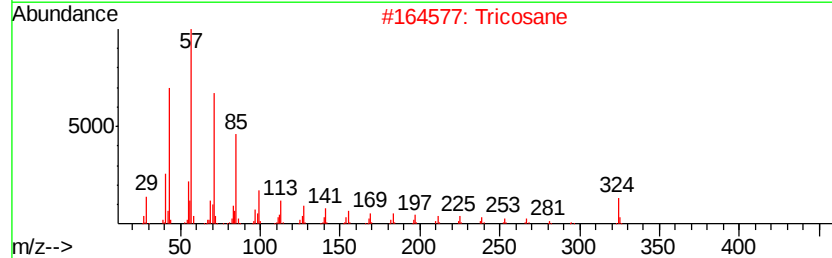
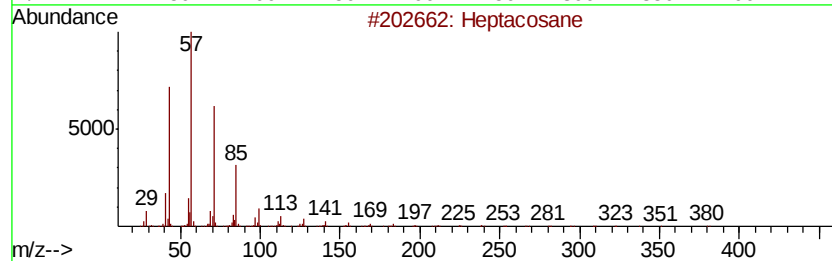
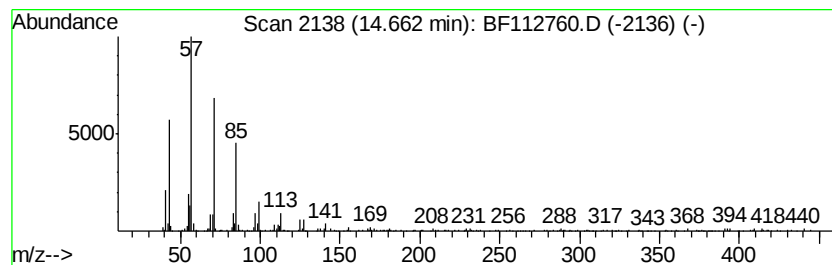
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	5.11 ng	258120	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	97
2		Tricosane	324	C23H48	000638-67-5	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Nonacosane	408	C29H60	000630-03-5	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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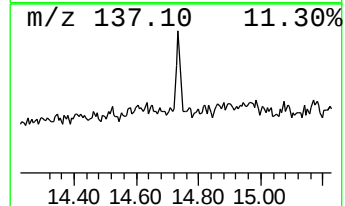
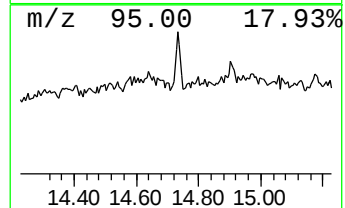
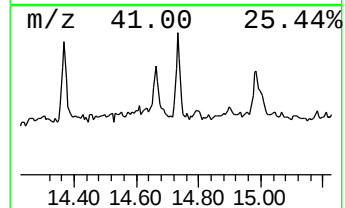
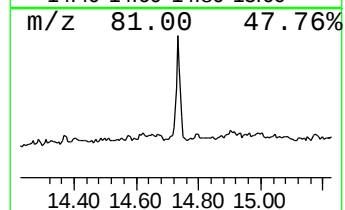
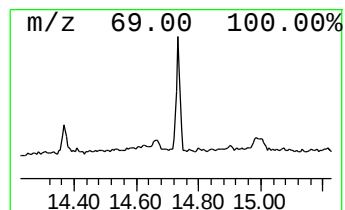
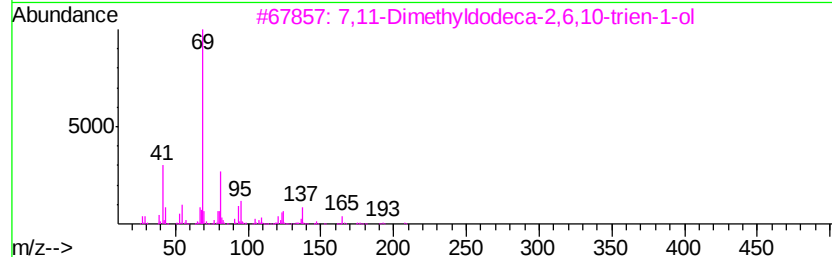
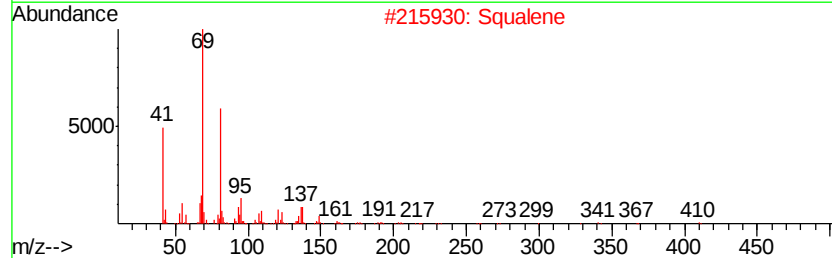
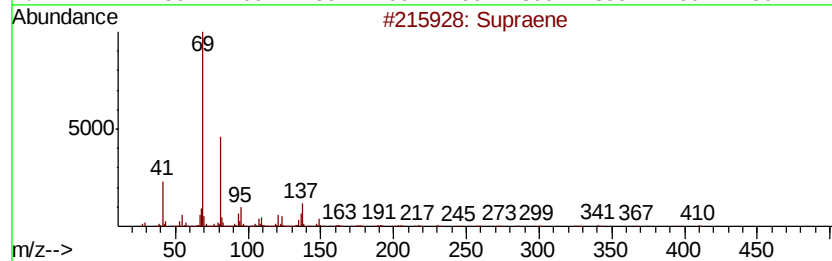
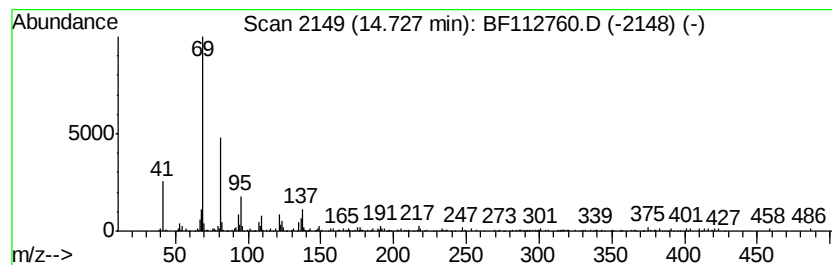
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.70 ng	237246	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	94
2		Squalene	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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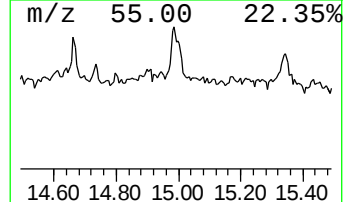
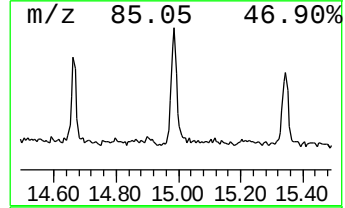
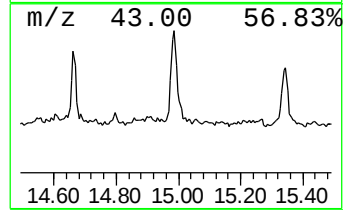
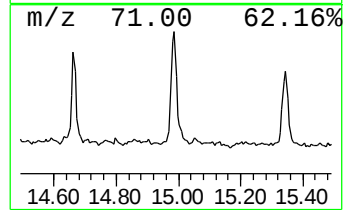
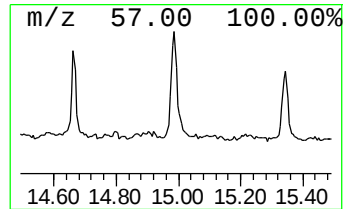
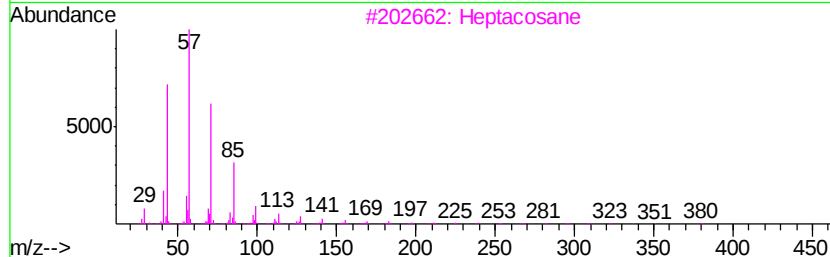
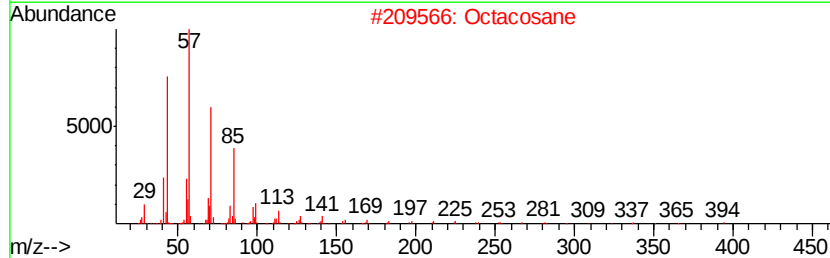
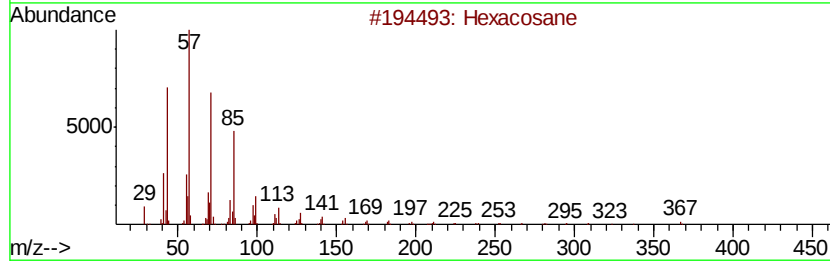
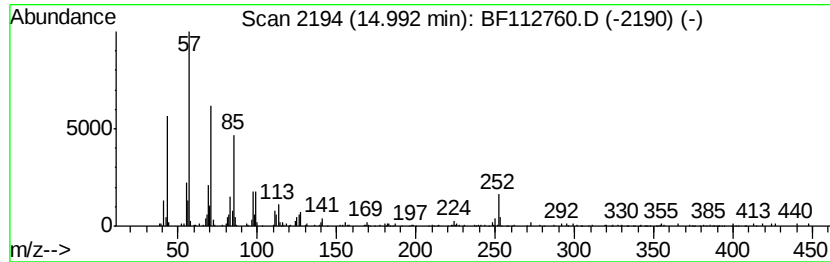
Instrument :
BNA_F
ClientSampleId :
BU-03-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.99	9.22 ng	465503	Perylene-d12		15.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptacosane	380	C27H56	000593-49-7	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Pentacosane	352	C25H52	000629-99-2	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112760.D
Acq On : 28 Feb 2019 14:15
Operator : JU/SJ
Sample : K1340-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

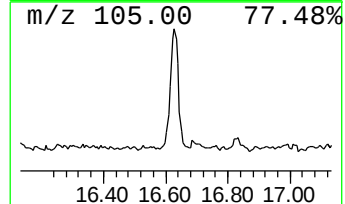
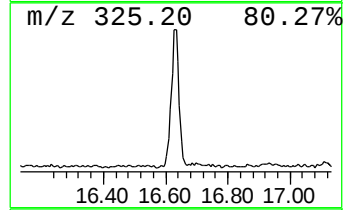
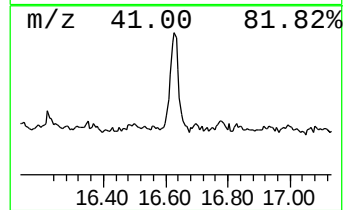
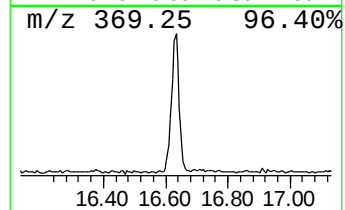
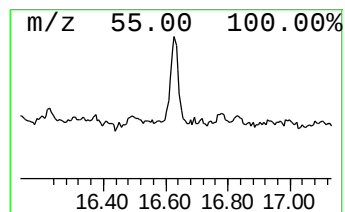
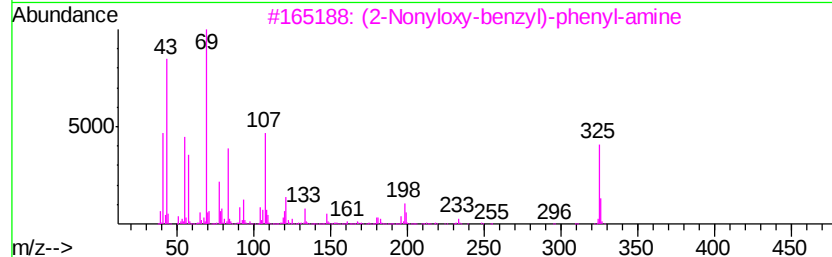
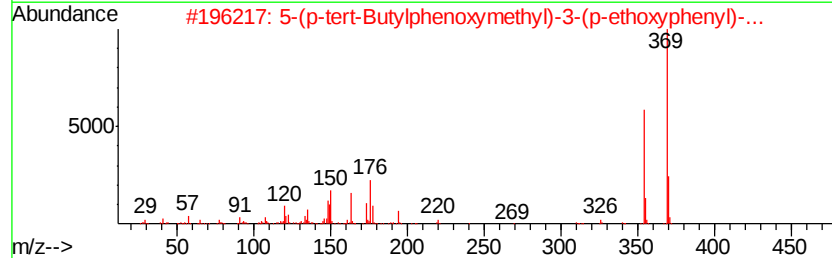
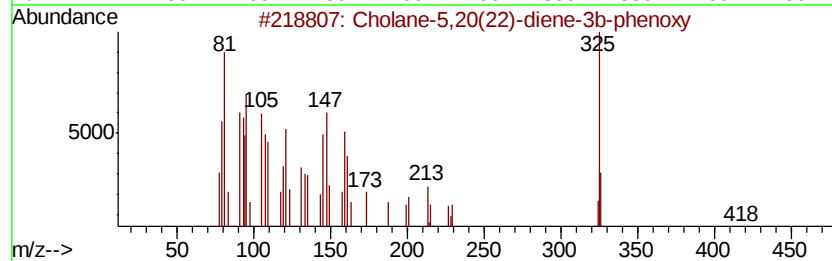
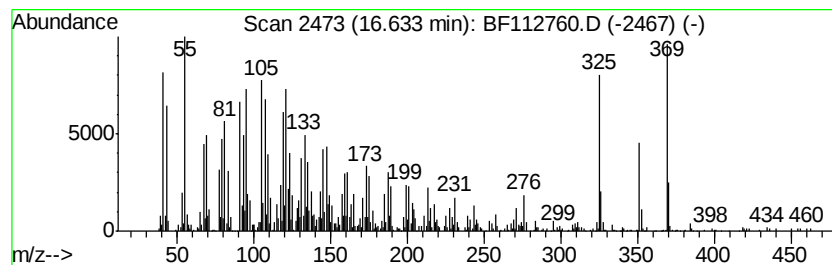
Instrument :
BNA_F
ClientSampleId :
BU-03-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.63	25.31 ng	1277700	Perylene-d12	15.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholane-5,20(22)-diene-3b-phenoxv	418	C30H42O	1000148-86-4	27
2		5-(p-tert-Butylphenoxyethyl)-3-...	369	C22H27NO4	005535-06-8	15
3		(2-Nonvloxy-benzyl)-phenyl-amine	325	C22H31NO	1000278-14-7	15
4		Benzyl 2-benzvloxyquinoline-4-ca...	369	C24H19NO3	1000242-75-3	11
5		1,3,5-Triazine-2,4-diamine, N,N'...	369	C21H19N7	033933-67-4	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
 Data File : BF112760.D
 Acq On : 28 Feb 2019 14:15
 Operator : JU/SJ
 Sample : K1340-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.52	6.52	70.0	ng	4289990	1	6.75	1226390	20.0
Caryophyllene	9.44	2.8	ng	228805	3	9.77	1618730	20.0
n-Hexadecanoic acid	11.79	9.0	ng	750222	4	11.25	1665290	20.0
9,12-Octadecadien...	12.34	4.4	ng	369607	4	11.25	1665290	20.0
9-Octadecenoic ac...	12.36	3.9	ng	327320	4	11.25	1665290	20.0
Octadecanoic acid	12.57	3.5	ng	267090	5	13.87	1527730	20.0
Cyclotetracosane	13.74	6.2	ng	476445	5	13.87	1527730	20.0
Heptadecane, 9-he...	14.06	2.0	ng	155255	5	13.87	1527730	20.0
Sulfurous acid, o...	14.37	4.6	ng	351064	5	13.87	1527730	20.0
Heptacosane	14.66	5.1	ng	258120	6	15.29	1009560	20.0
Supraene	14.73	4.7	ng	237246	6	15.29	1009560	20.0
Hexacosane	14.99	9.2	ng	465503	6	15.29	1009560	20.0
unknown16.63	16.63	25.3	ng	1277700	6	15.29	1009560	20.0