

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
 Data File : BF112874.D
 Acq On : 6 Mar 2019 1:32
 Operator : JU/SJ
 Sample : K1705-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EXT-028-SW005-022719

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	558	rBV	3242374	3005216	85.69%	8.078%
2	6.381	724	730	740	rBV	2950843	3352953	95.60%	9.012%
3	6.510	747	752	755	rBV	3674824	3311232	94.41%	8.900%
4	6.739	787	791	800	rBV	1221511	970913	27.68%	2.610%
5	6.898	814	818	821	rBV	2789535	2467647	70.36%	6.633%
6	7.298	881	886	889	rBV	2148456	1998157	56.97%	5.371%
7	8.022	1005	1009	1031	rBV	1217509	1232262	35.13%	3.312%
8	9.098	1188	1192	1206	rBV	3430306	3129636	89.23%	8.412%
9	9.486	1255	1258	1264	rVB	180035	183019	5.22%	0.492%
10	9.769	1302	1306	1315	rBV	1316063	1256650	35.83%	3.378%
11	10.557	1435	1440	1449	rBV	2077505	2117871	60.39%	5.693%
12	11.251	1554	1558	1561	rBV	1183436	1204108	34.33%	3.236%
13	11.786	1645	1649	1652	rBV2	389908	378611	10.80%	1.018%
14	11.816	1652	1654	1659	rVB	71919	73750	2.10%	0.198%
15	12.069	1694	1697	1703	rVB	35229	44111	1.26%	0.119%
16	12.457	1759	1763	1767	rBV	330756	308922	8.81%	0.830%
17	12.568	1779	1782	1787	rBV2	114192	141040	4.02%	0.379%
18	12.680	1796	1801	1807	rBV	287121	300709	8.57%	0.808%
19	12.827	1822	1826	1830	rBV	2697146	2633756	75.09%	7.079%
20	13.116	1871	1875	1882	rVB3	39802	58891	1.68%	0.158%
21	13.304	1904	1907	1914	rVB2	42767	69330	1.98%	0.186%
22	13.504	1937	1941	1945	rBV	3543188	3507241	100.00%	9.427%
23	13.627	1958	1962	1964	rBV2	33220	42592	1.21%	0.114%
24	13.733	1975	1980	1986	rBV3	271107	380705	10.85%	1.023%
25	13.874	1999	2004	2007	rBV2	1536822	1611697	45.95%	4.332%
26	13.898	2007	2008	2014	rVB	195471	158632	4.52%	0.426%
27	14.057	2032	2035	2039	rBV2	126371	119375	3.40%	0.321%
28	14.362	2083	2087	2093	rBV	244080	276924	7.90%	0.744%
29	14.657	2134	2137	2144	rVB	229318	226169	6.45%	0.608%
30	14.886	2173	2176	2179	rBV	132563	176930	5.04%	0.476%
31	14.974	2188	2191	2202	rVB	264959	372237	10.61%	1.001%
32	15.168	2221	2224	2228	rBV	75762	91604	2.61%	0.246%
33	15.227	2230	2234	2238	rVV	85649	122628	3.50%	0.330%
34	15.286	2239	2244	2248	rVV	758477	951609	27.13%	2.558%

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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	15.333	2249	2252	2256	rVB	197751	238986	6.81%	0.642%
36	15.739	2317	2321	2326	rBV	171538	245088	6.99%	0.659%
37	16.121	2381	2386	2395	rBV3	240981	443244	12.64%	1.191%

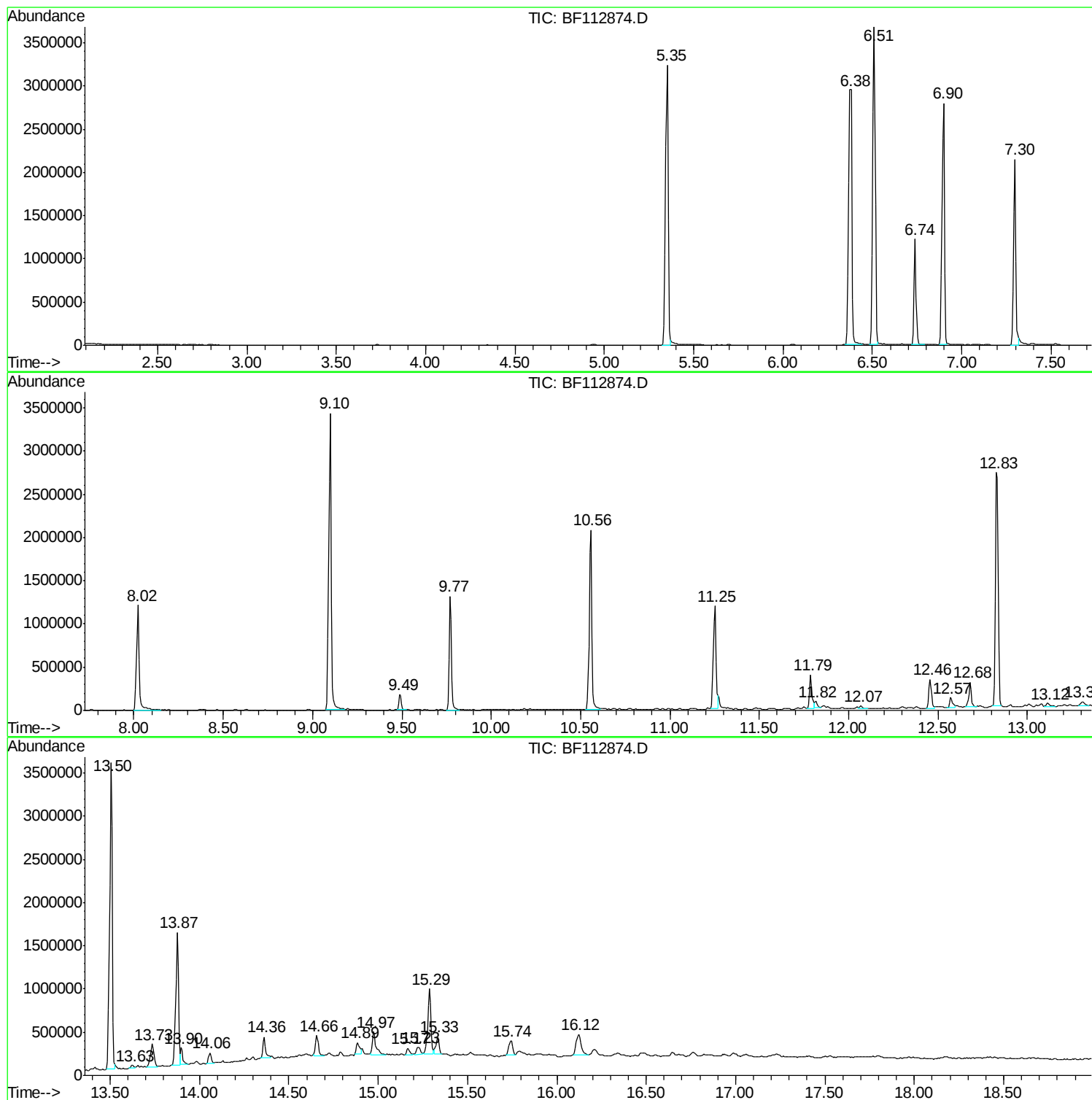
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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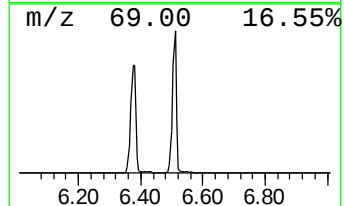
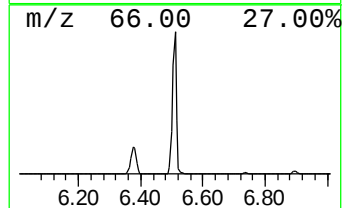
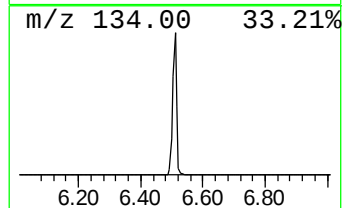
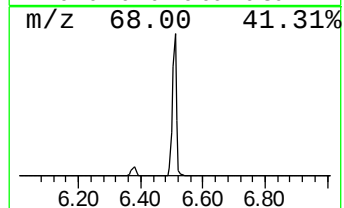
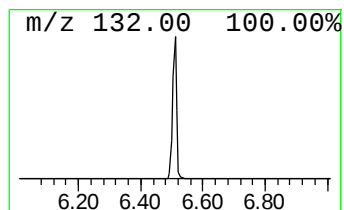
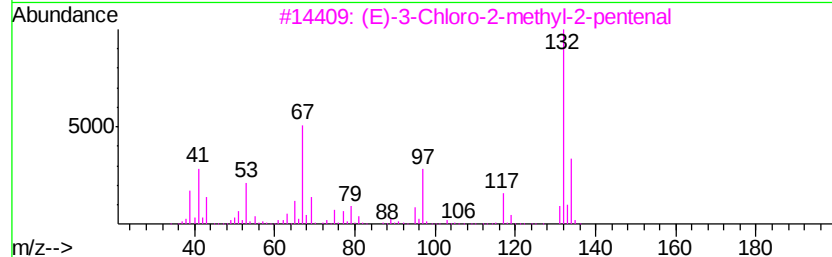
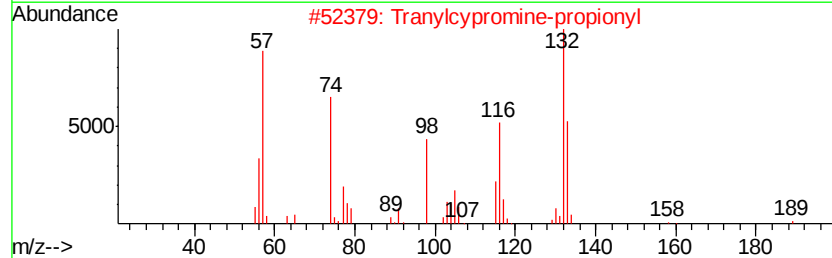
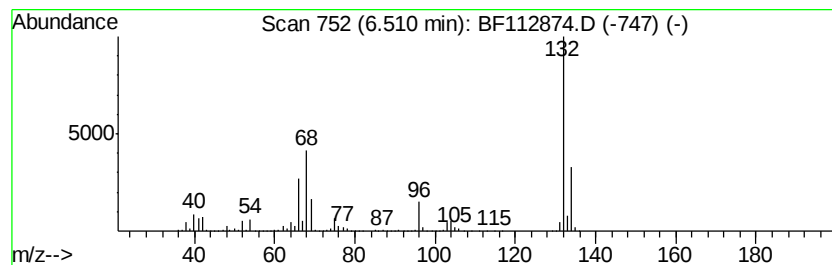
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	68.21 ng	3311230	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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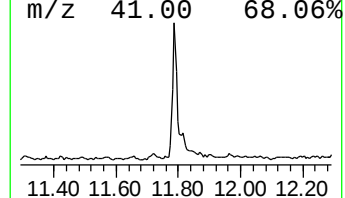
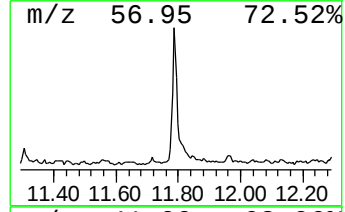
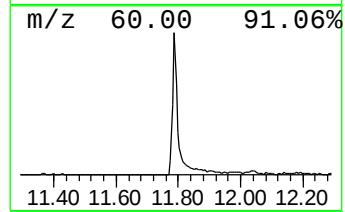
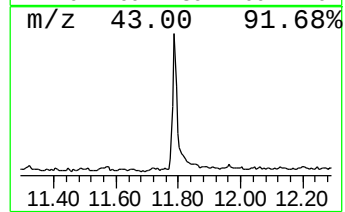
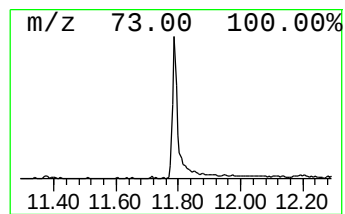
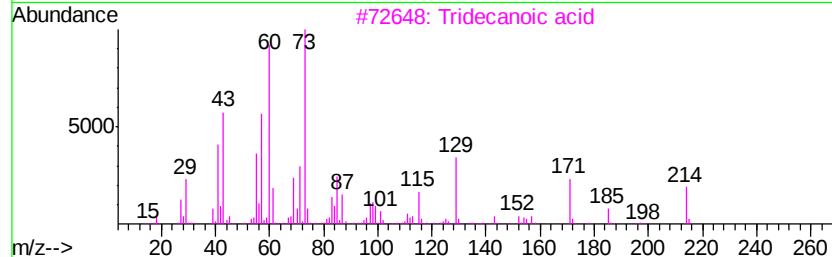
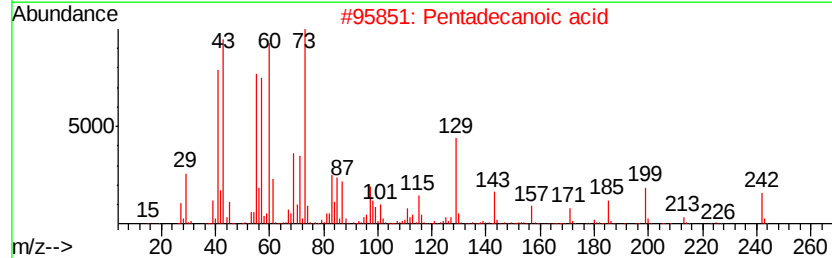
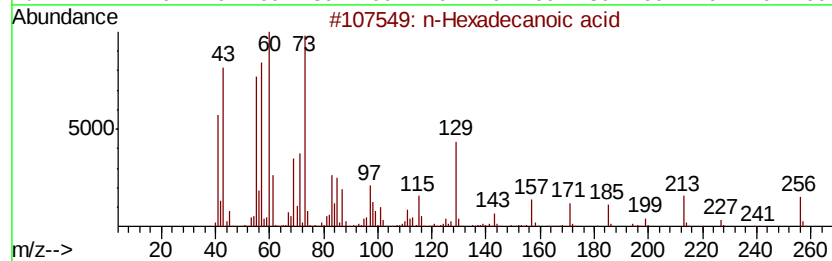
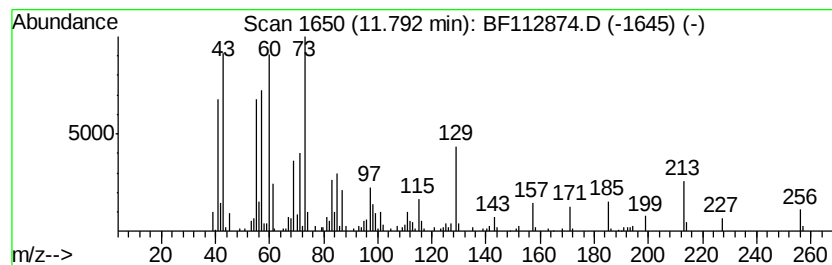
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.79	6.29 ng	378611	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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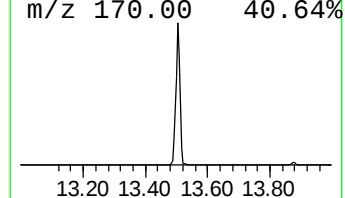
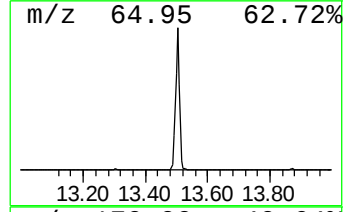
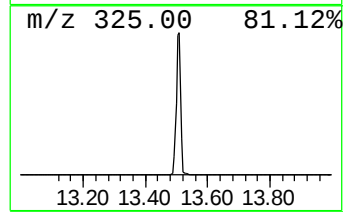
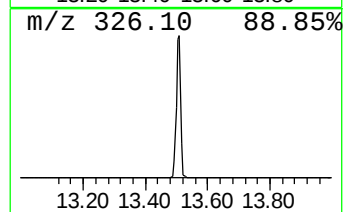
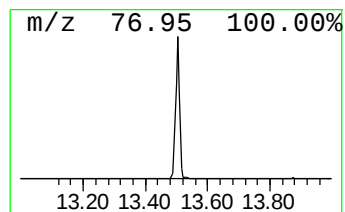
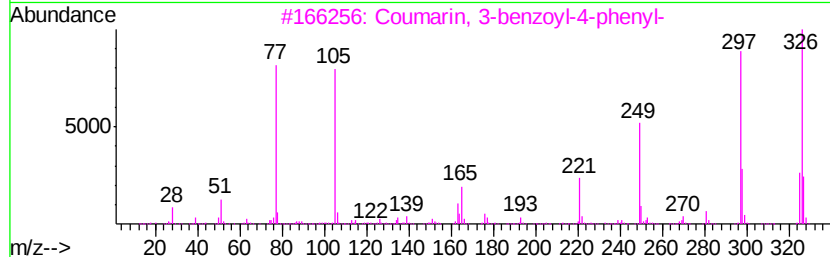
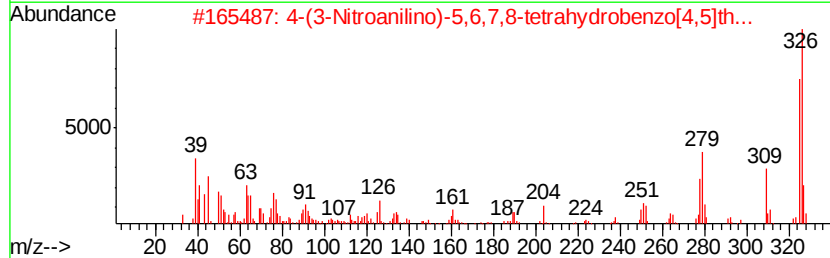
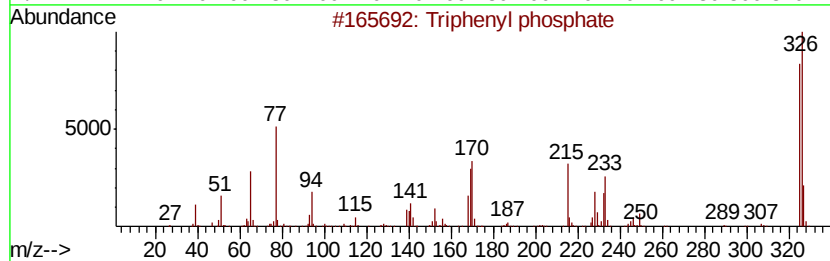
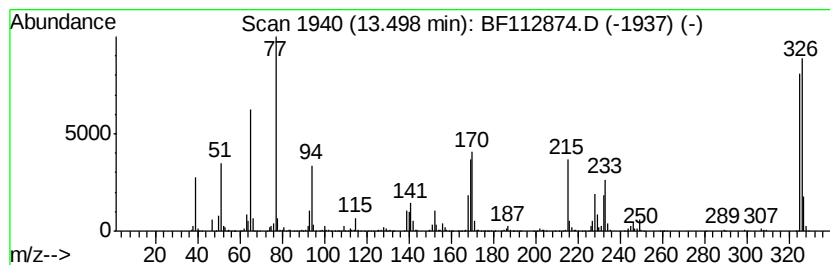
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Triphenyl phosphate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	43.52 ng	3507240	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triphenyl phosphate	326	C18H15O4P	000115-86-6	99
2		4-(3-Nitroanilino)-5,6,7,8-tetra...	326	C16H14N4O2S	313952-58-8	12
3		Coumarin, 3-benzoyl-4-phenyl-	326	C22H14O3	019725-29-2	12
4		(1-Allyl-2-oxo-1,2-dihydro-indol...	326	C20H14N4O	1000296-28-1	12
5		3-Buten-2-one, 4-(2-furanyl)-	136	C8H8O2	000623-15-4	10



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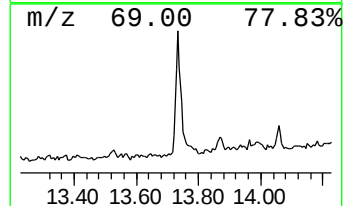
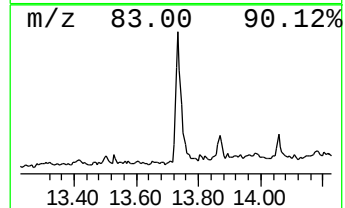
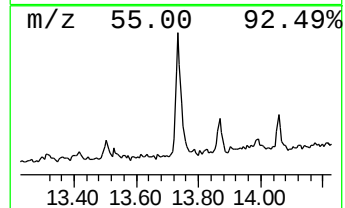
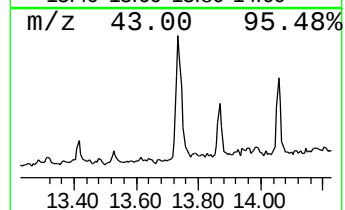
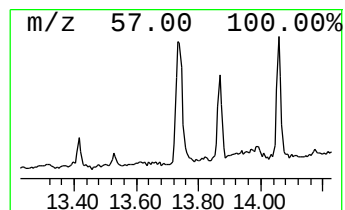
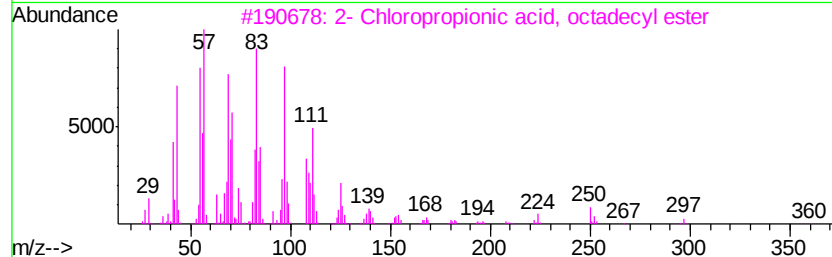
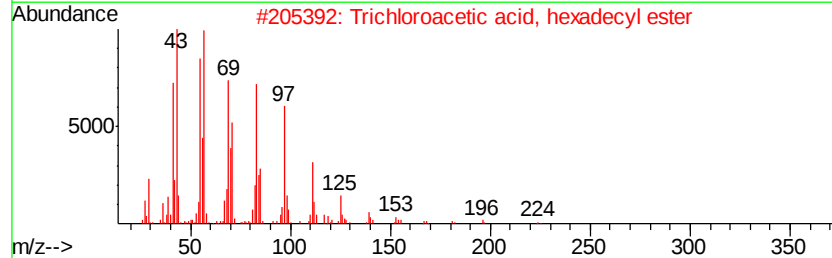
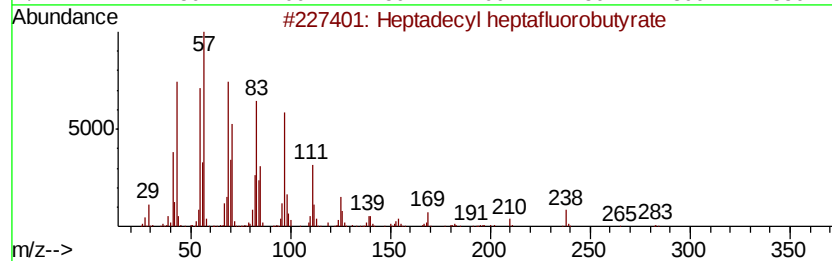
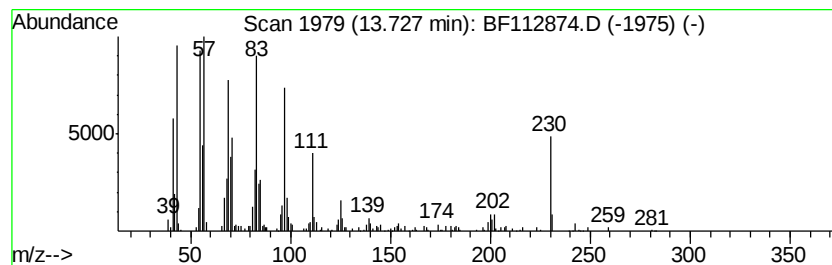
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 Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	4.72 ng	380705	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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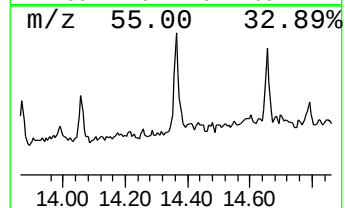
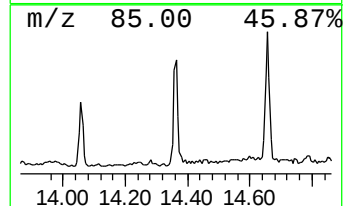
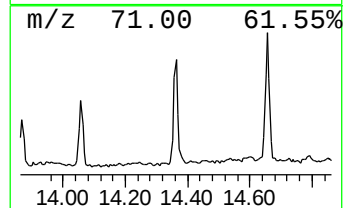
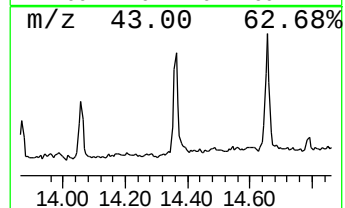
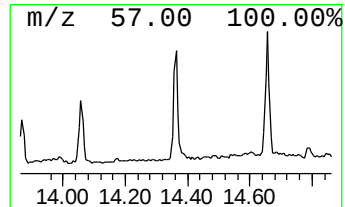
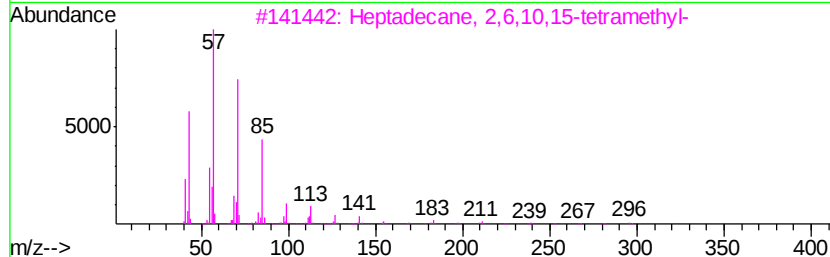
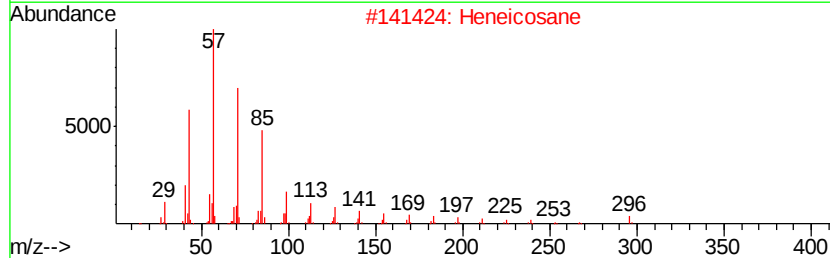
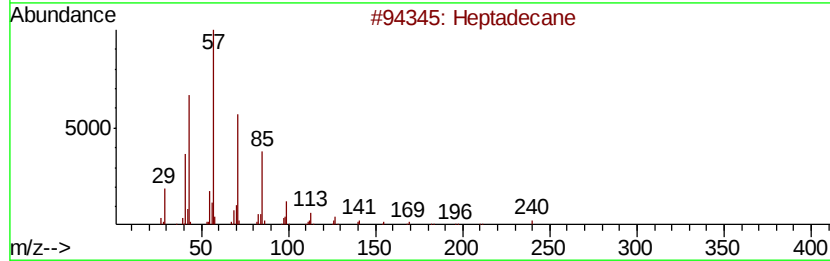
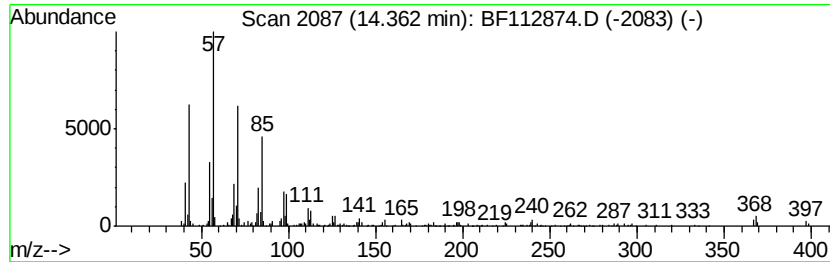
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Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.44 ng	276924	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	96
2	Heneicosane	296 C21H44	000629-94-7	96
3	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	93
4	Tritetracontane	605 C43H88	007098-21-7	90
5	Heptacosane, 1-chloro-	414 C27H55Cl	062016-79-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112874.D
Acq On : 6 Mar 2019 1:32
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-028-SW005-022719

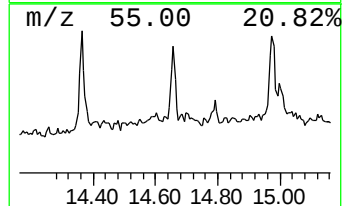
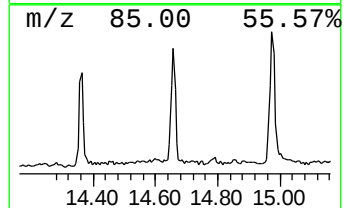
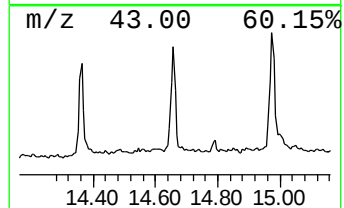
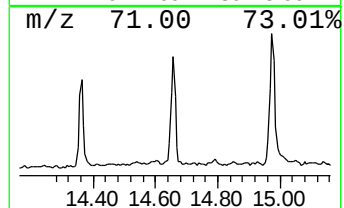
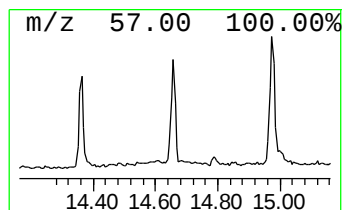
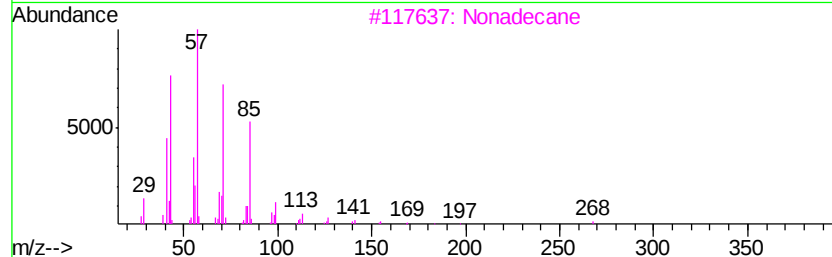
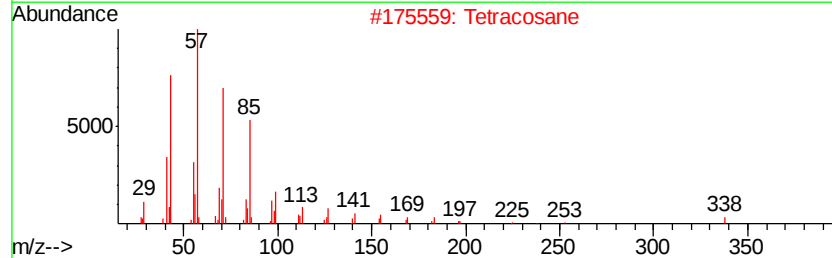
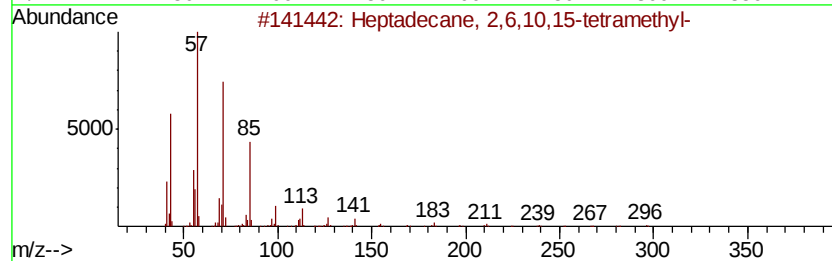
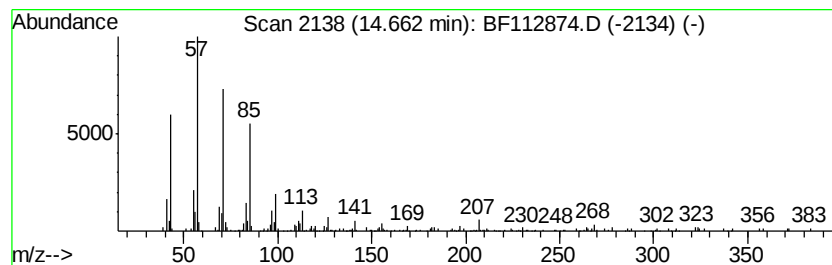
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	4.75 ng	226169	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Tetracosane	338	C24H50	000646-31-1	87
3		Nonadecane	268	C19H40	000629-92-5	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112874.D
Acq On : 6 Mar 2019 1:32
Operator : JU/SJ
Sample : K1705-04
Misc :
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Instrument :
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ClientSampleId :
EXT-028-SW005-022719

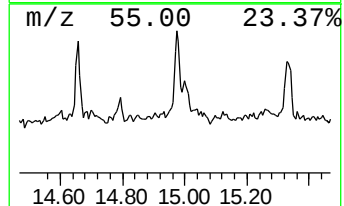
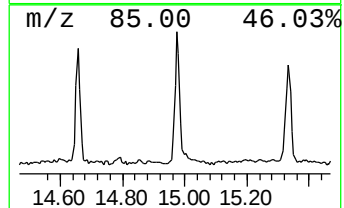
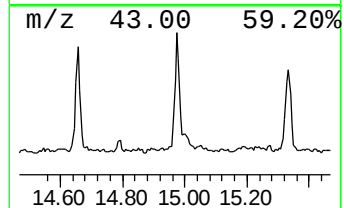
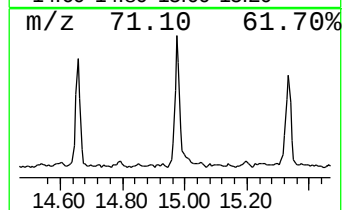
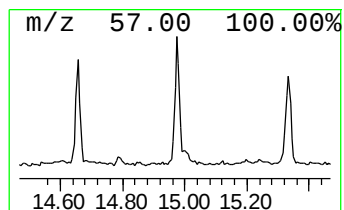
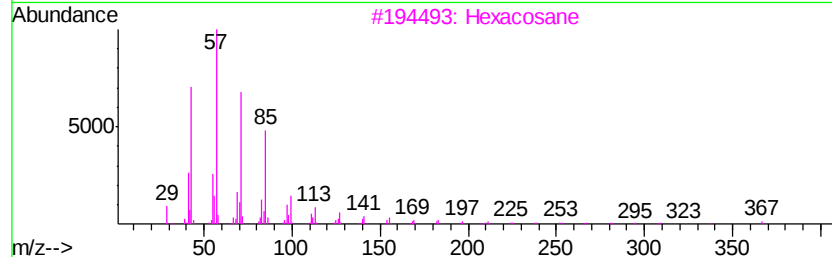
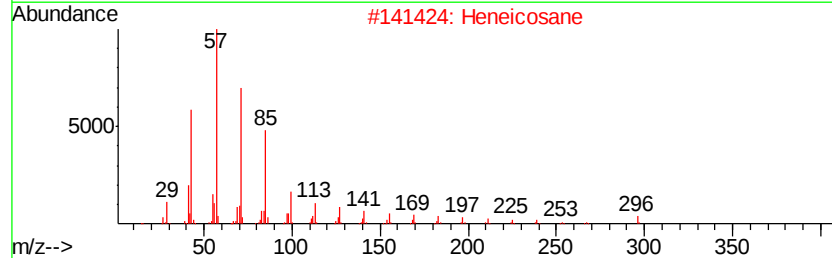
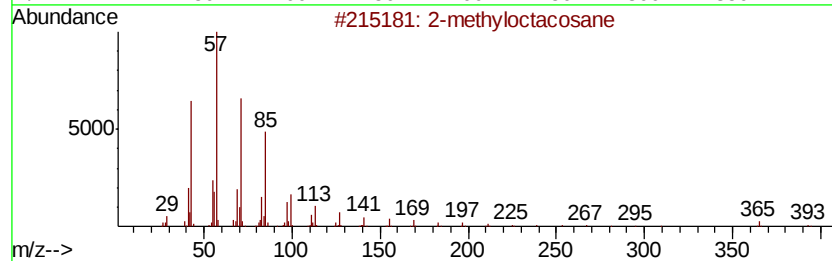
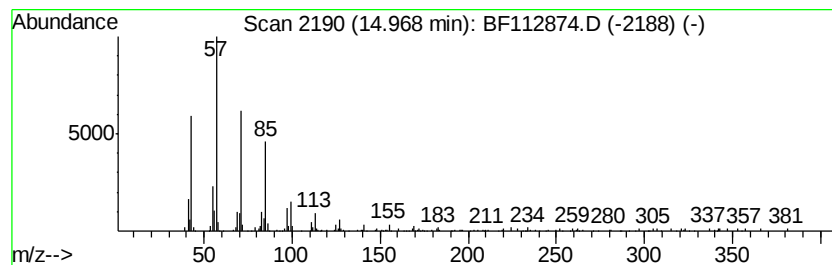
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	7.82 ng	372237	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	87
2		Heneicosane	296	C21H44	000629-94-7	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112874.D
Acq On : 6 Mar 2019 1:32
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

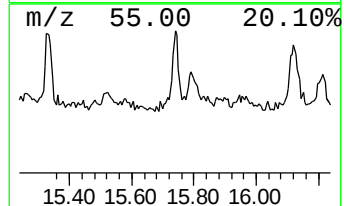
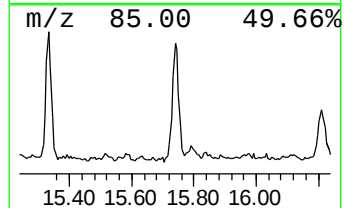
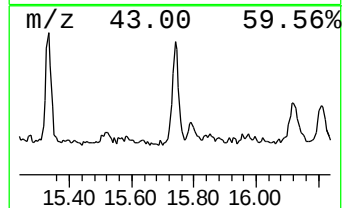
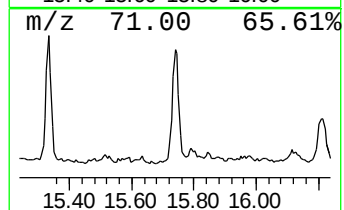
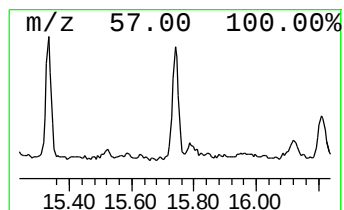
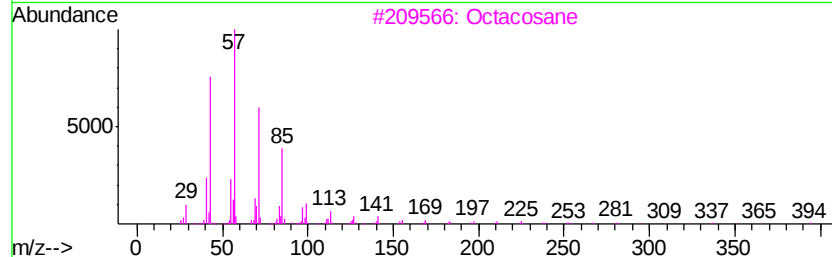
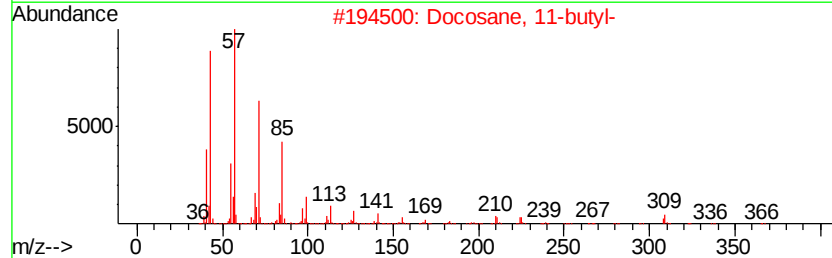
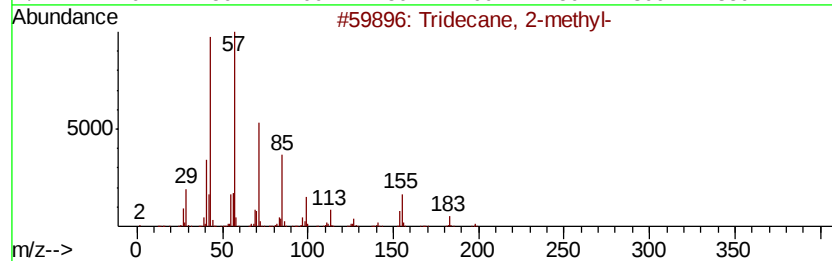
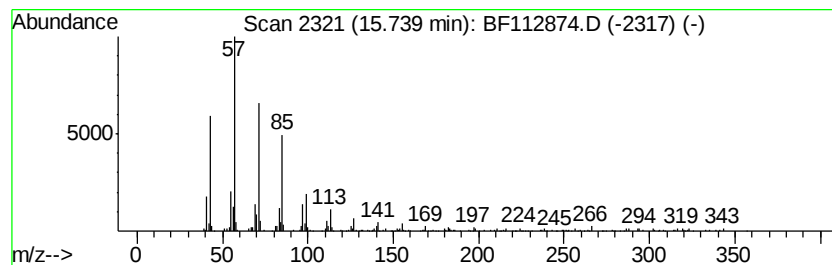
Instrument :
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ClientSampleId :
EXT-028-SW005-022719

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 9 Tridecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.74	5.15 ng	245088	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
3	Octacosane	394	C28H58	000630-02-4	70
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	68
5	Heptacosane	380	C27H56	000593-49-7	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112874.D
Acq On : 6 Mar 2019 1:32
Operator : JU/SJ
Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

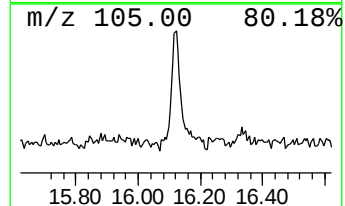
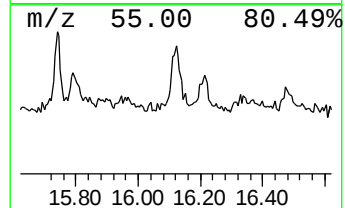
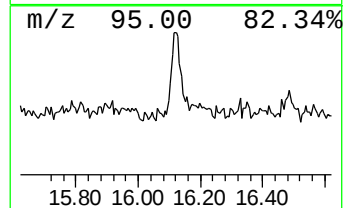
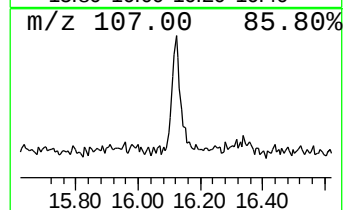
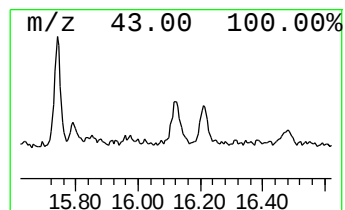
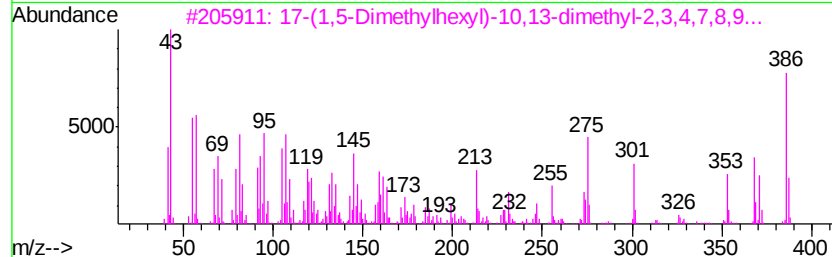
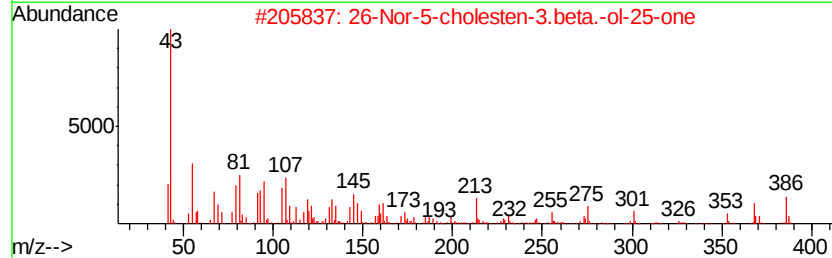
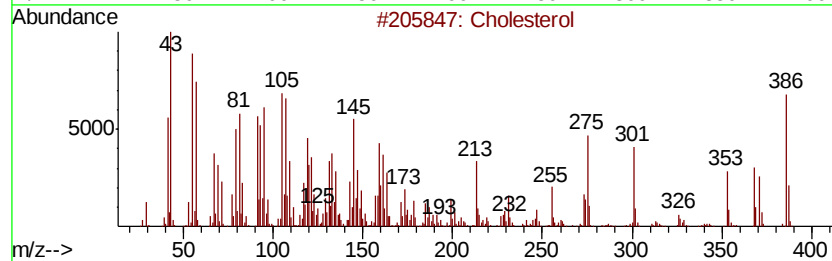
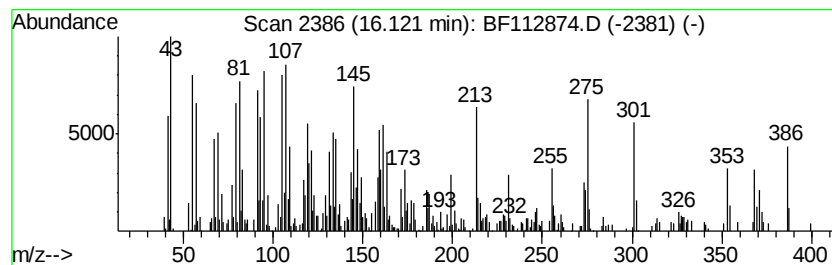
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cholesterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.12	9.32 ng	443244	Perylene-d12	15.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholesterol	386	C27H46O	000057-88-5	99
2		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3		17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	94
4		Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	72
5		Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
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Sample : K1705-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic acid	11.79	6.3	ng	378611	4	11.25	1204110	20.0
Triphenyl phosphate	13.50	43.5	ng	3507240	5	13.87	1611700	20.0
Heptadecyl heptaf...	13.73	4.7	ng	380705	5	13.87	1611700	20.0
Heptadecane	14.36	3.4	ng	276924	5	13.87	1611700	20.0
Heptadecane, 2,6,...	14.66	4.8	ng	226169	6	15.29	951609	20.0
2-methyloctacosane	14.97	7.8	ng	372237	6	15.29	951609	20.0
Tridecane, 2-methyl-	15.74	5.2	ng	245088	6	15.29	951609	20.0
Cholesterol	16.12	9.3	ng	443244	6	15.29	951609	20.0