

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
 Data File : BF118007.D
 Acq On : 26 Nov 2019 15:16
 Operator : JU
 Sample : K5840-09 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-SE-01

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-BF111319.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	2.140	4	9	22	rVB	284945	375233	31.55%	2.391%
2	5.093	507	511	523	rVB	182284	183173	15.40%	1.167%
3	5.504	577	581	584	rBV	1061390	954867	80.29%	6.084%
4	6.516	749	753	769	rBV	1228527	1064608	89.51%	6.783%
5	6.663	774	778	781	rBV	1151022	1061318	89.24%	6.762%
6	6.893	814	817	821	rBV	872610	684011	57.51%	4.358%
7	7.051	840	844	847	rBV	1085316	855208	71.91%	5.449%
8	7.451	908	912	917	rBV	725004	601028	50.54%	3.829%
9	8.181	1033	1036	1039	rBV	1041952	799525	67.22%	5.094%
10	8.204	1039	1040	1043	rVB	37019	20073	1.69%	0.128%
11	8.239	1043	1046	1049	rVB	20984	17829	1.50%	0.114%
12	8.598	1105	1107	1110	rVB	17802	14105	1.19%	0.090%
13	8.769	1134	1136	1139	rBV	39337	34514	2.90%	0.220%
14	9.086	1188	1190	1196	rVB4	10265	14075	1.18%	0.090%
15	9.257	1216	1219	1225	rBV	1472658	1148641	96.58%	7.318%
16	9.339	1230	1233	1235	rBV	51293	40768	3.43%	0.260%
17	9.651	1283	1286	1290	rVB	124131	100852	8.48%	0.643%
18	9.869	1318	1323	1329	rVB2	26614	28885	2.43%	0.184%
19	9.945	1332	1336	1339	rBV	1031138	842084	70.80%	5.365%
20	10.139	1365	1369	1374	rBV5	14450	23556	1.98%	0.150%
21	10.345	1401	1404	1406	rBV3	15051	15246	1.28%	0.097%
22	10.369	1406	1408	1411	rVB	26827	22876	1.92%	0.146%
23	10.592	1441	1446	1449	rBV2	15019	20129	1.69%	0.128%
24	10.733	1466	1470	1482	rVB	775929	652399	54.85%	4.157%
25	10.845	1487	1489	1490	rBV	24851	17840	1.50%	0.114%
26	11.298	1563	1566	1569	rBV	18899	23630	1.99%	0.151%
27	11.328	1569	1571	1576	rVB3	15122	16561	1.39%	0.106%
28	11.439	1586	1590	1593	rBV	1023168	917394	77.14%	5.845%
29	11.675	1627	1630	1633	rBV5	11047	14085	1.18%	0.090%
30	11.957	1675	1678	1683	rBV	194059	183170	15.40%	1.167%
31	12.133	1705	1708	1713	rVB	31937	27206	2.29%	0.173%
32	12.522	1772	1774	1777	rBV2	34050	35070	2.95%	0.223%
33	12.627	1787	1792	1794	rBV5	21620	40016	3.36%	0.255%
34	12.657	1794	1797	1798	rBV	31774	32988	2.77%	0.210%

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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	12.745	1809	1812	1819	rBV4	54723	80197	6.74%	0.511%
36	12.839	1826	1828	1831	rBV4	14891	15673	1.32%	0.100%
37	12.898	1834	1838	1843	rVB2	58461	77228	6.49%	0.492%
38	13.022	1856	1859	1863	rBV	1352182	1189330	100.00%	7.577%
39	13.104	1868	1873	1875	rBV5	33674	69089	5.81%	0.440%
40	13.251	1895	1898	1902	rBV	83247	93432	7.86%	0.595%
41	13.327	1909	1911	1912	rBV2	31004	29485	2.48%	0.188%
42	13.598	1955	1957	1960	rBV	115726	91843	7.72%	0.585%
43	13.763	1981	1985	1986	rBV4	42641	57494	4.83%	0.366%
44	13.927	2010	2013	2020	rBV3	147875	231967	19.50%	1.478%
45	14.086	2037	2040	2044	rBV	946652	812330	68.30%	5.175%
46	14.245	2065	2067	2070	rVB	138657	113690	9.56%	0.724%
47	14.551	2117	2119	2122	rVB	132773	105895	8.90%	0.675%
48	14.868	2170	2173	2177	rVB	137364	152453	12.82%	0.971%
49	15.215	2229	2232	2236	rBV	158739	198662	16.70%	1.266%
50	15.592	2292	2296	2305	rVB2	602267	1122755	94.40%	7.153%
51	15.892	2344	2347	2352	rBV6	67570	151129	12.71%	0.963%
52	16.074	2375	2378	2384	rVB	117848	149817	12.60%	0.955%
53	17.433	2605	2609	2610	rBV4	53348	70391	5.92%	0.448%

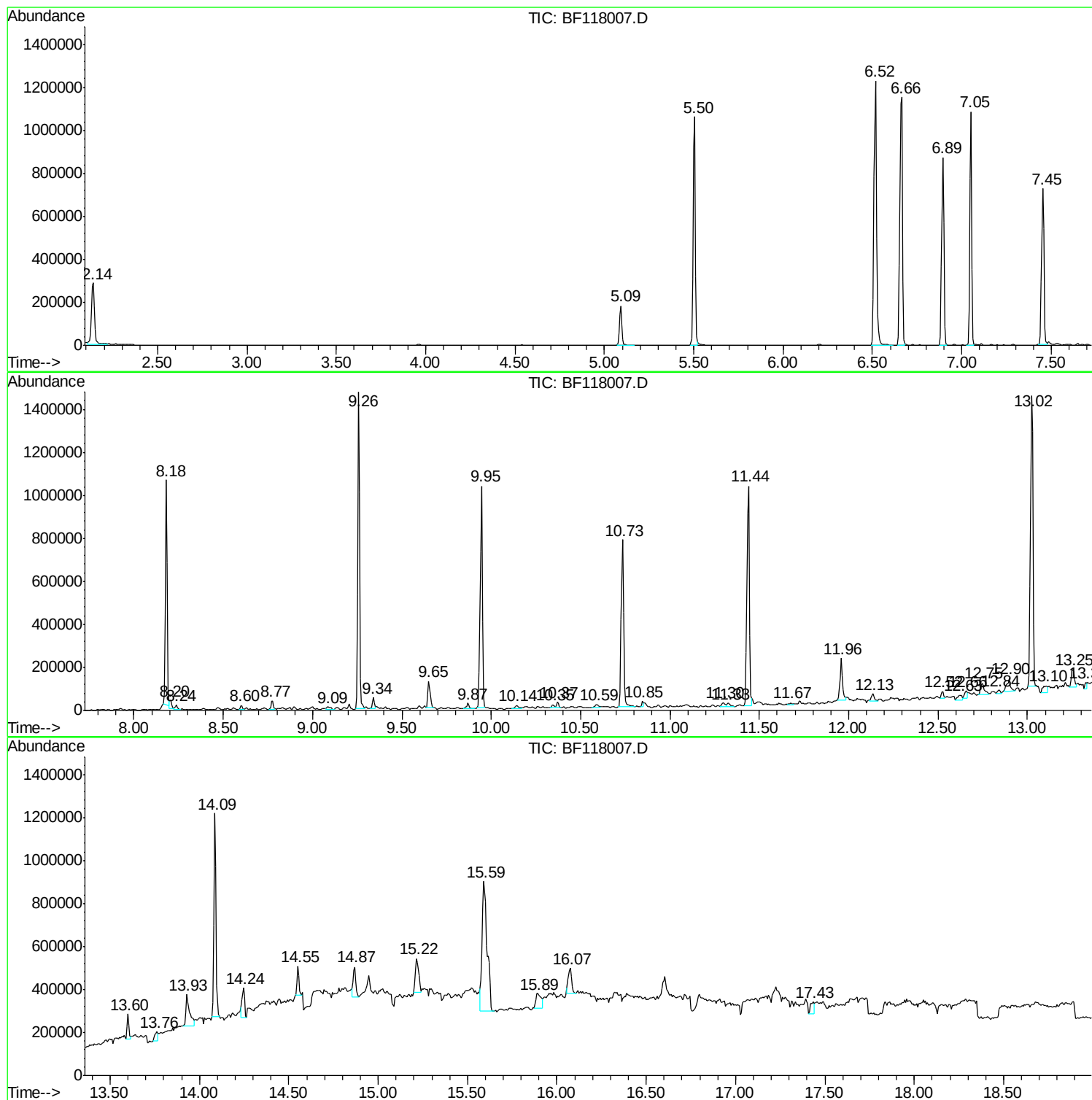
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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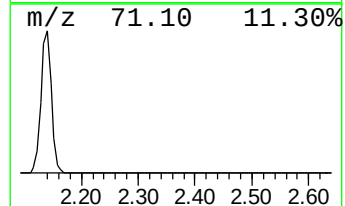
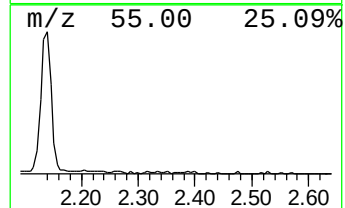
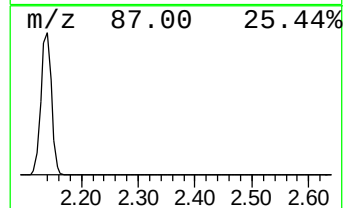
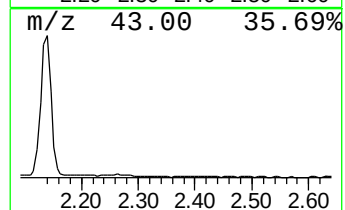
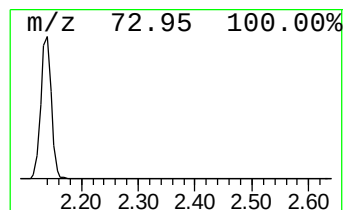
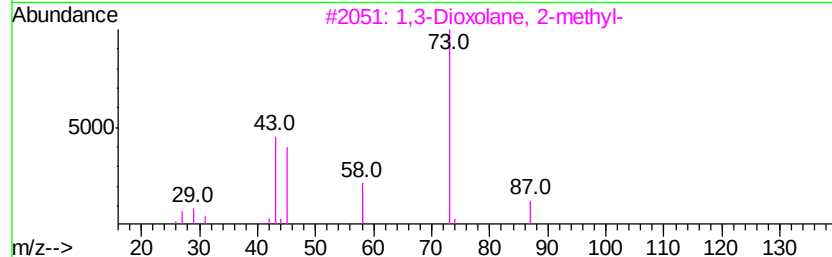
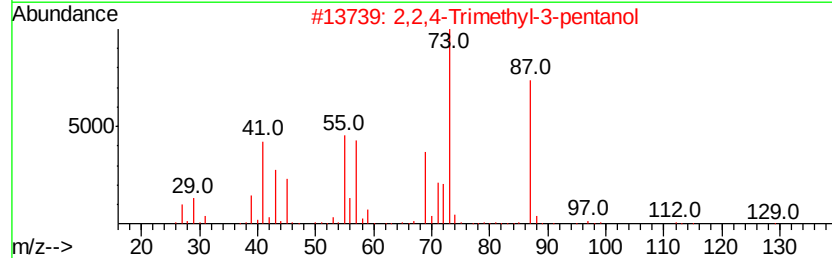
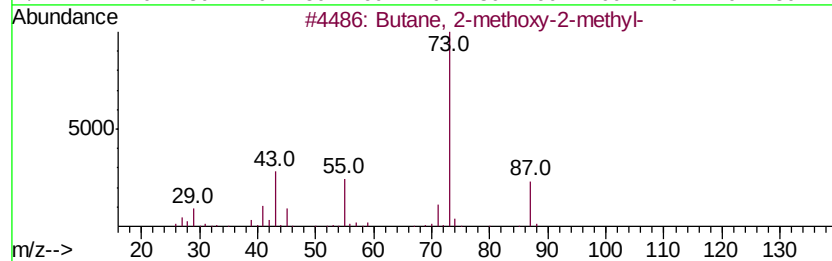
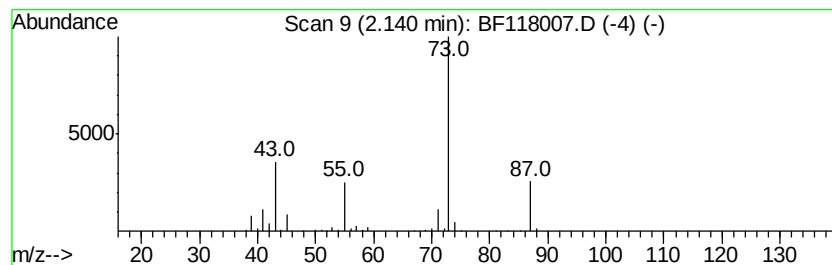
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	10.97 ng	375233	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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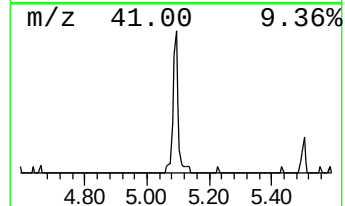
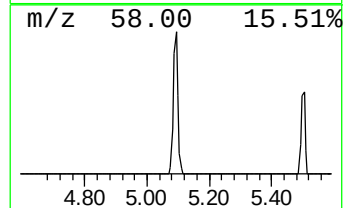
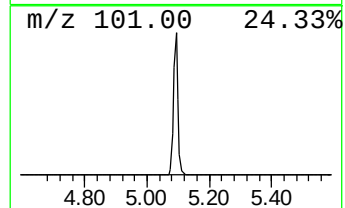
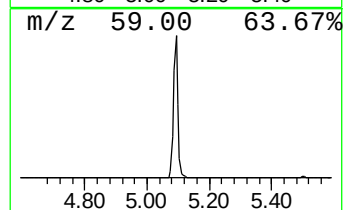
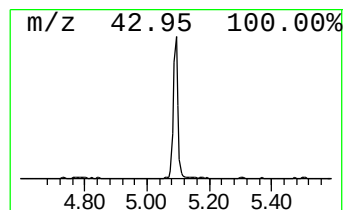
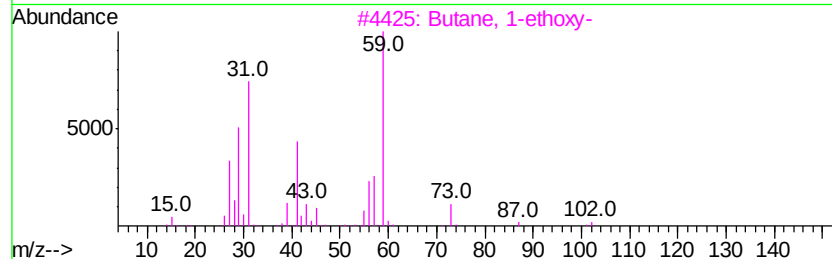
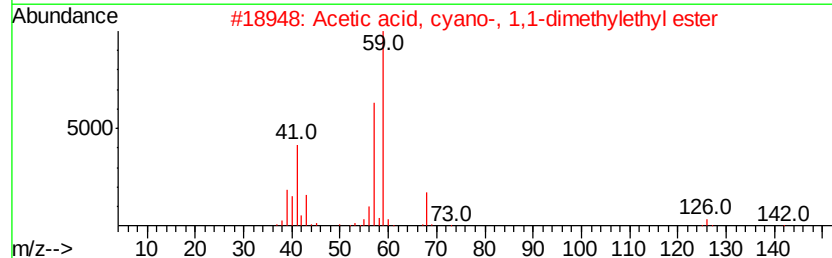
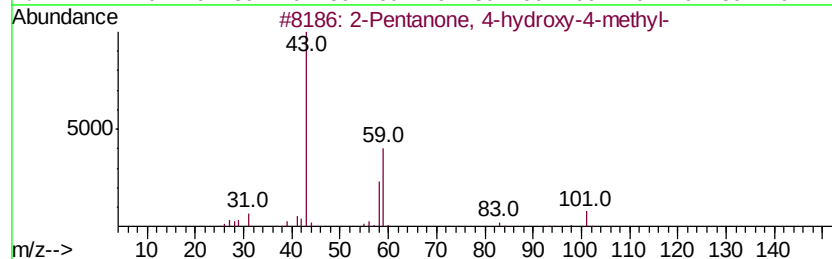
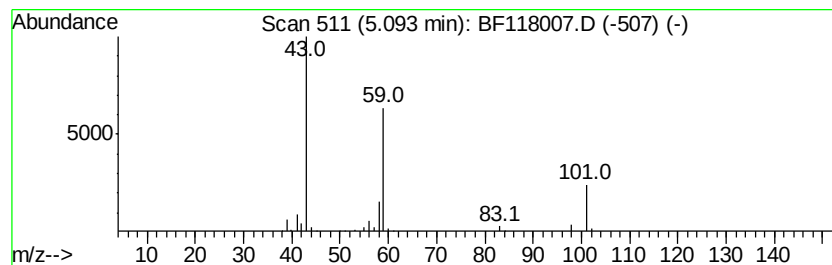
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.36 ng	183173	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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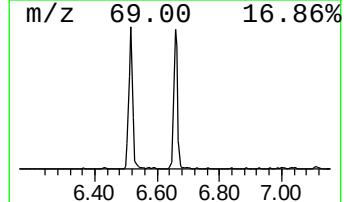
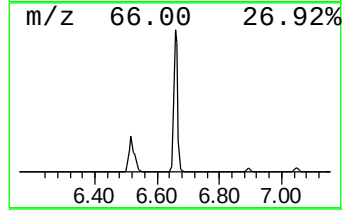
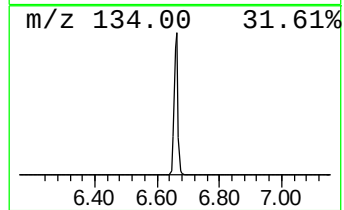
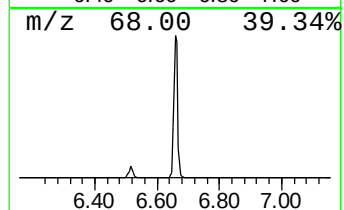
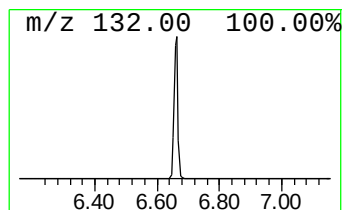
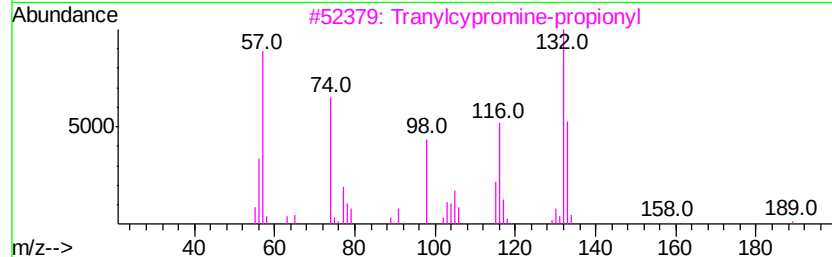
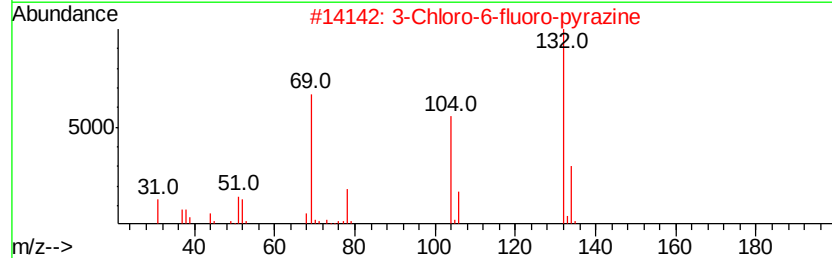
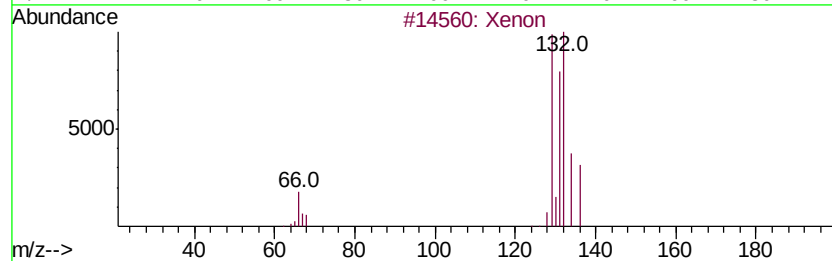
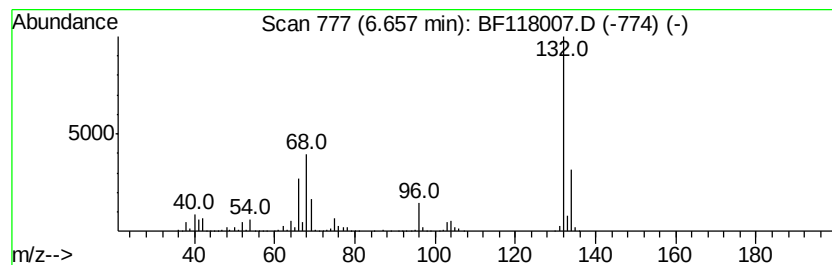
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Peak Number 3 Xenon Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	31.03 ng	1061320	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Xenon	132	Xe	007440-63-3	50
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranvlcyppromine-propionyl	189	C12H15NO	1000123-86-3	16
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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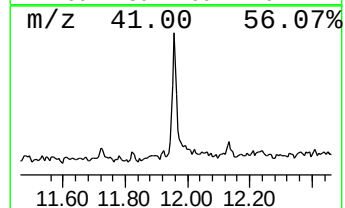
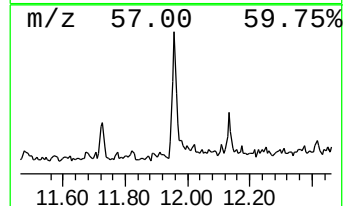
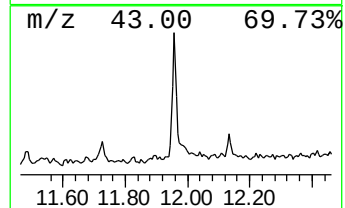
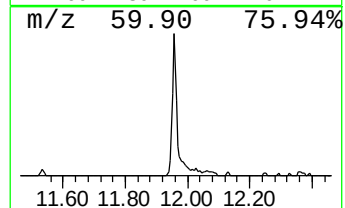
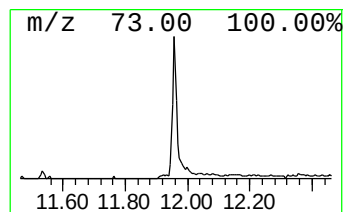
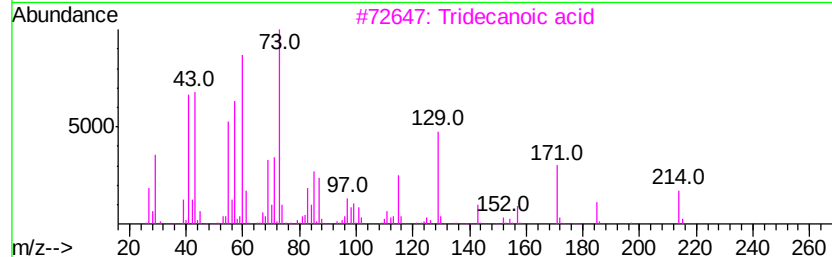
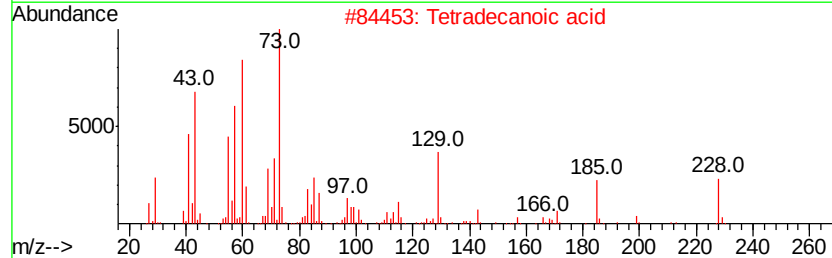
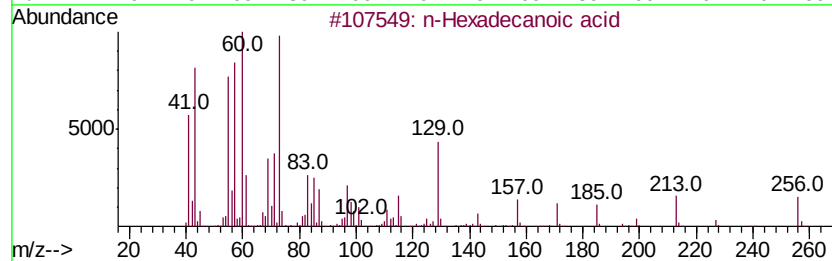
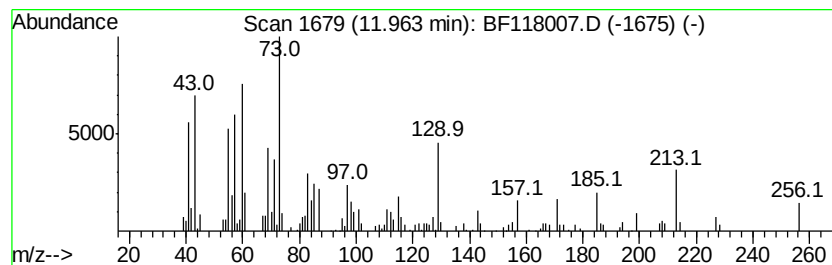
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.96	3.99 ng	183170	Phenanthrene-d10	11.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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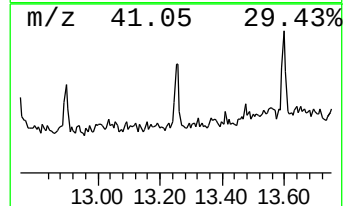
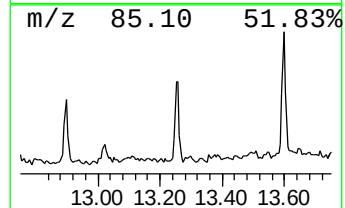
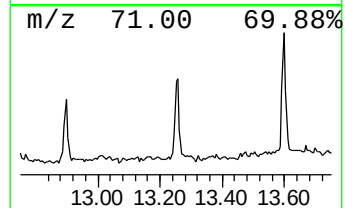
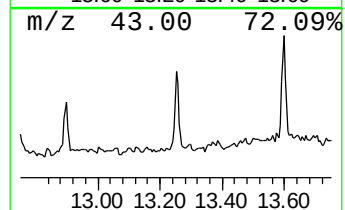
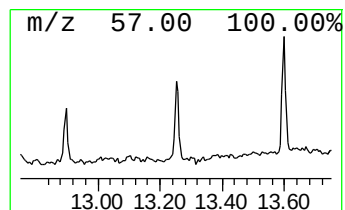
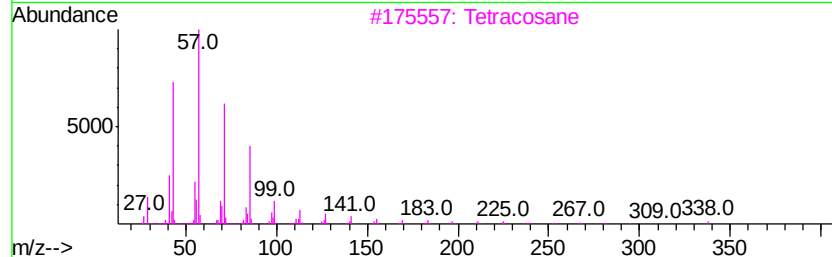
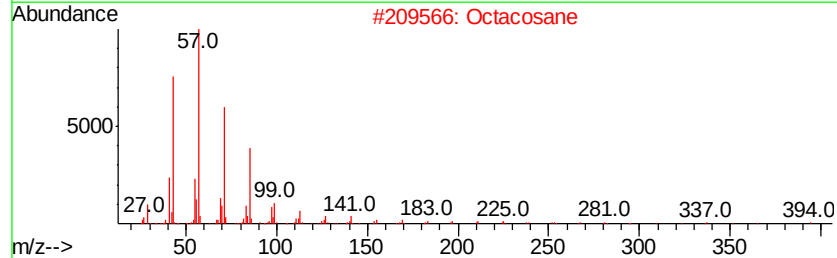
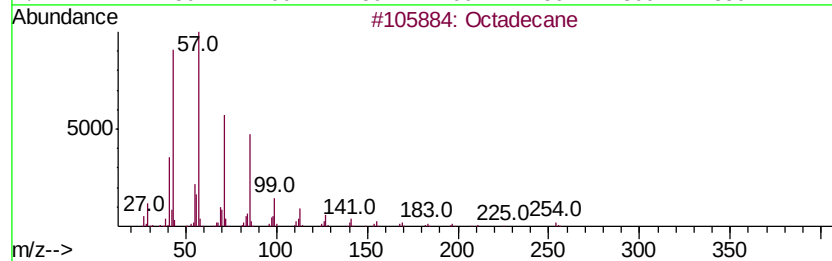
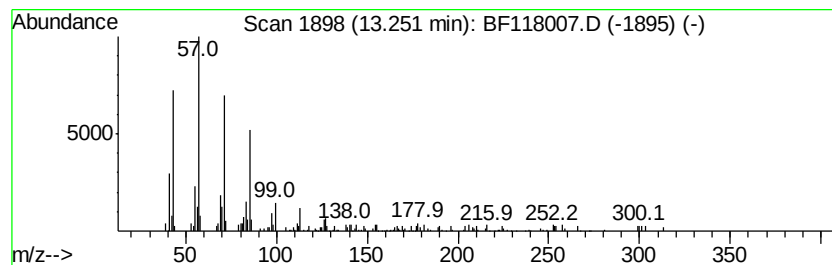
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	2.30 ng	93432	Chrysene-d12	14.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	93
2	Octacosane	394 C28H58	000630-02-4	90
3	Tetracosane	338 C24H50	000646-31-1	87
4	Heneicosane	296 C21H44	000629-94-7	87
5	Heptadecane	240 C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118007.D
Acq On : 26 Nov 2019 15:16
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

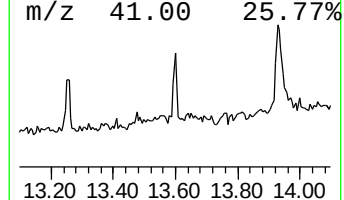
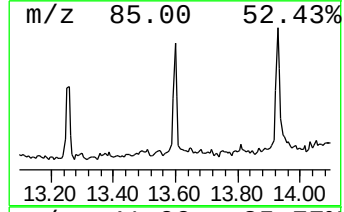
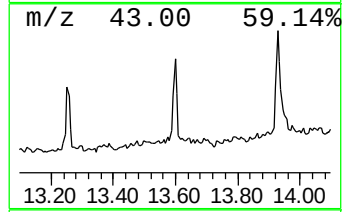
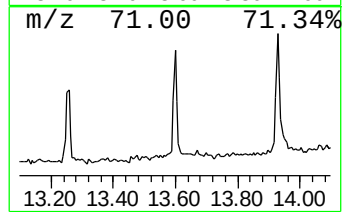
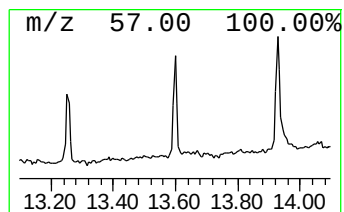
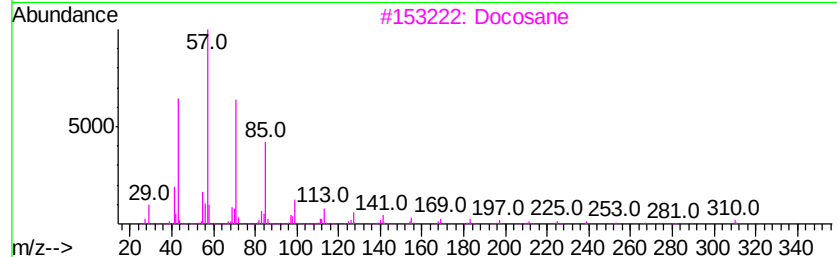
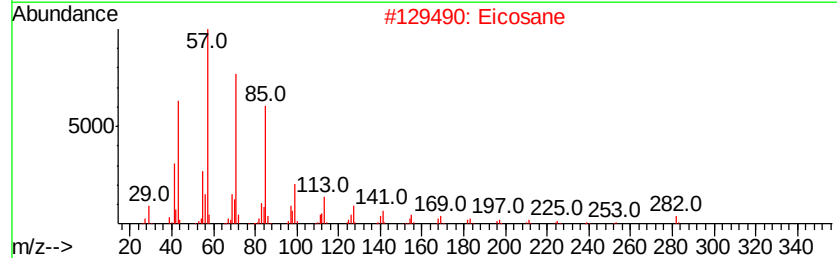
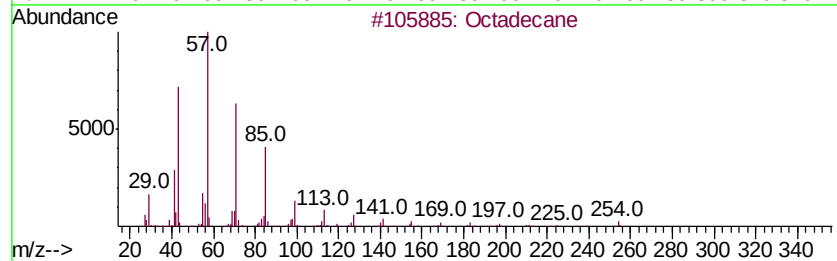
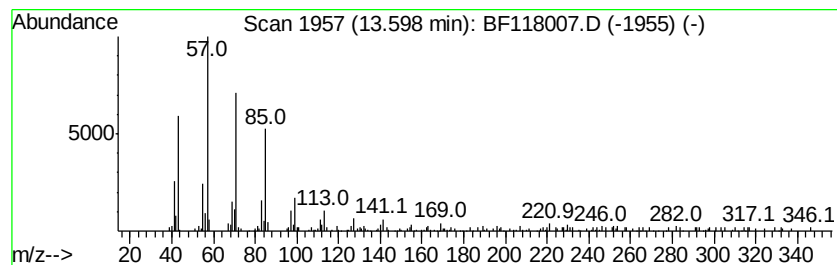
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.60	2.26 ng	91843	Chrysene-d12		14.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Eicosane	282	C20H42	000112-95-8	94
3	Docosane	310	C22H46	000629-97-0	93
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Tetradecane	198	C14H30	000629-59-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
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Sample : K5840-09 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

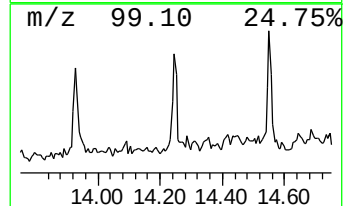
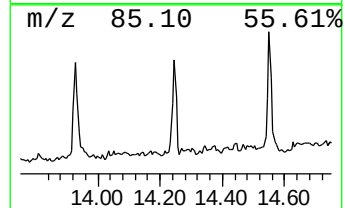
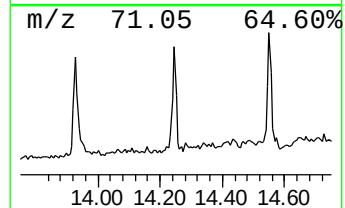
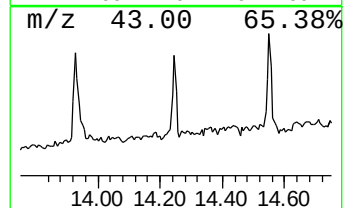
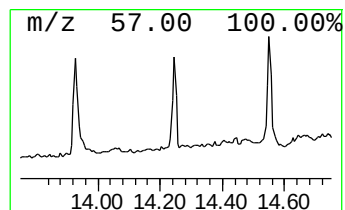
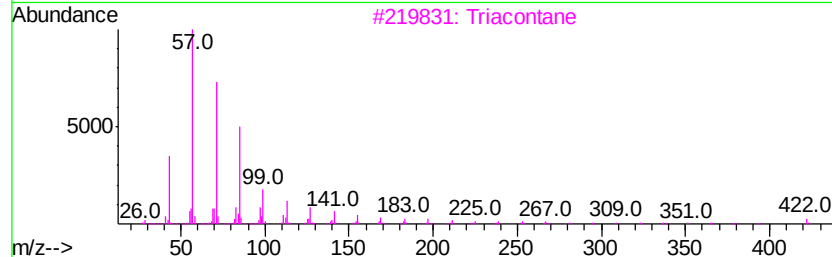
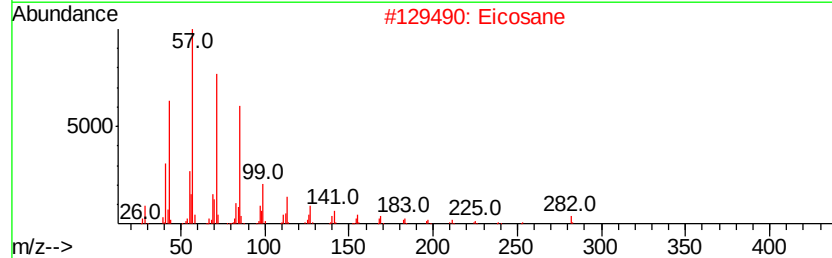
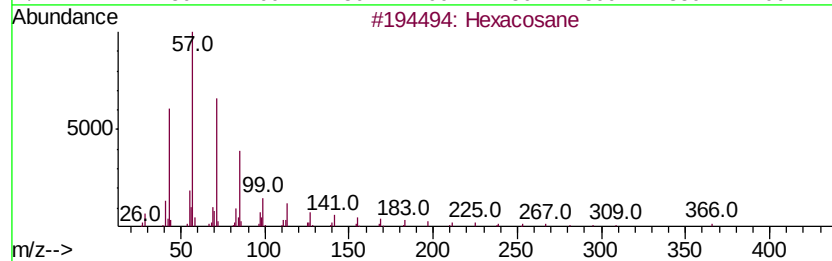
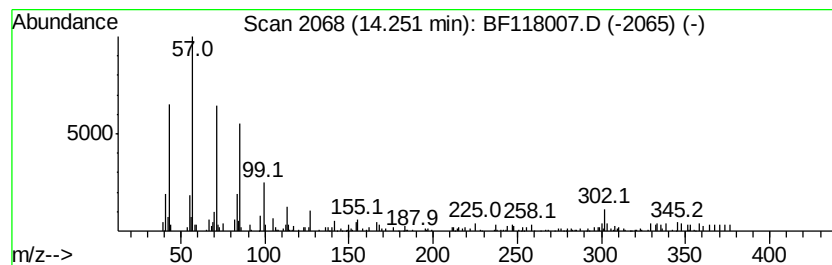
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.80 ng	113690	Chrysene-d12	14.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	93
2	Eicosane	282 C20H42	000112-95-8	93
3	Triacontane	422 C30H62	000638-68-6	86
4	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
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Sample : K5840-09 2X
Misc :
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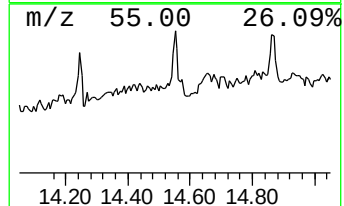
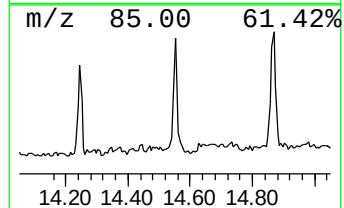
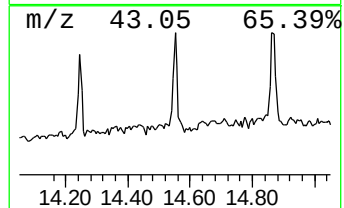
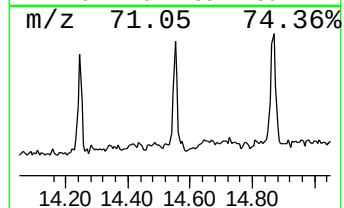
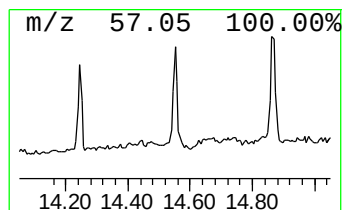
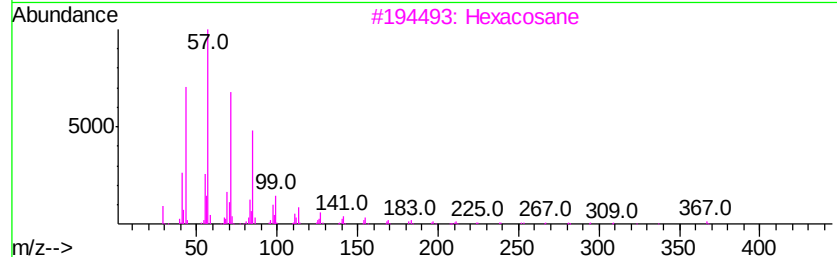
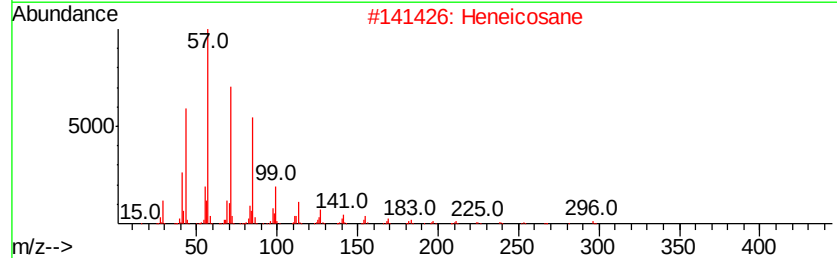
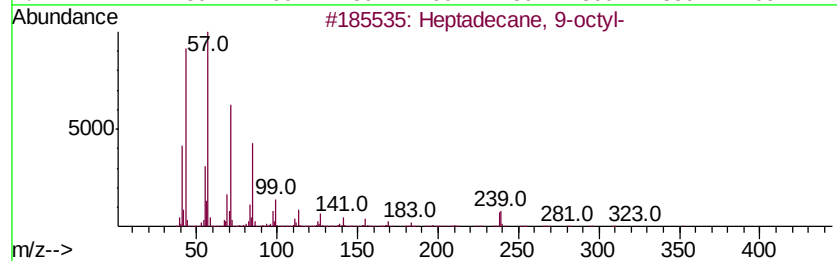
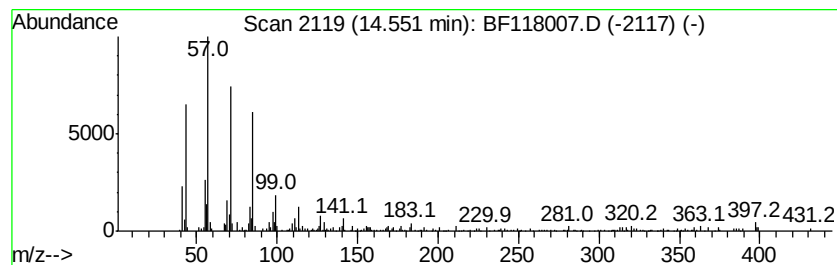
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.55	2.61 ng	105895	Chrysene-d12		14.09	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Heneicosane	296	C21H44	000629-94-7	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
 Data File : BF118007.D
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Instrument :
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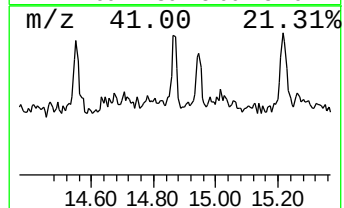
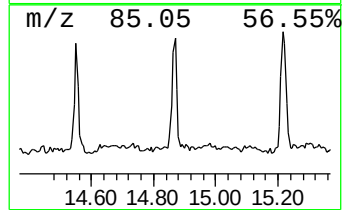
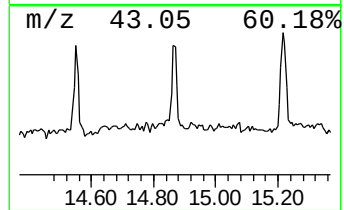
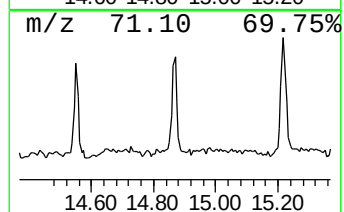
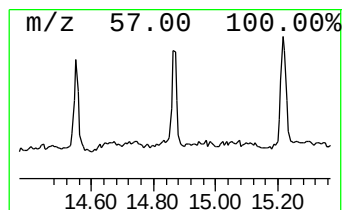
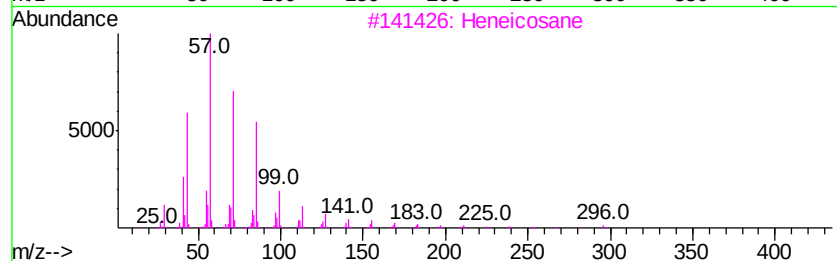
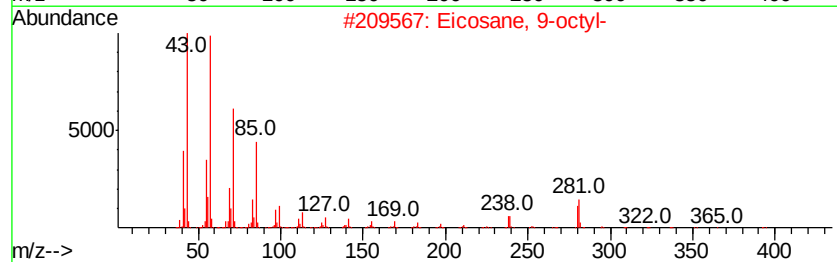
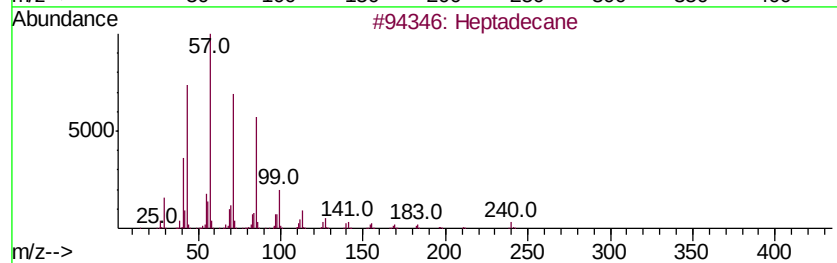
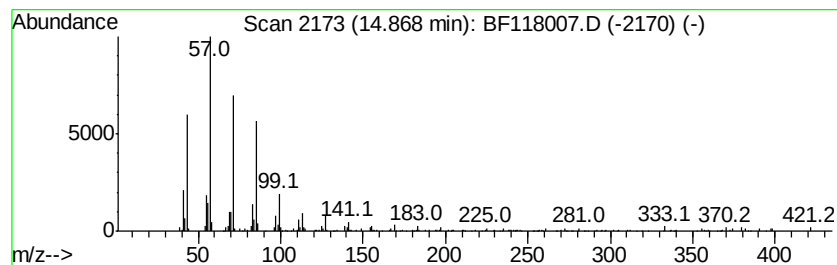
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.72 ng	152453	Perylene-d12	15.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Eicosane, 9-octyl-		394	C28H58	013475-77-9	87
3	Heneicosane		296	C21H44	000629-94-7	87
4	Octadecane		254	C18H38	000593-45-3	80
5	Heneicosane, 11-pentyl-		366	C26H54	014739-72-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
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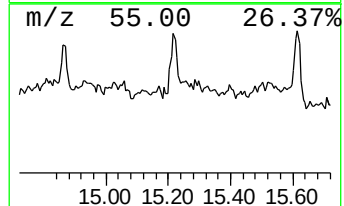
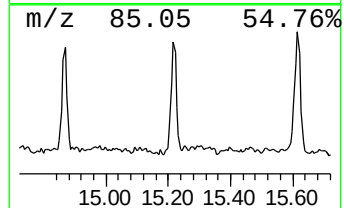
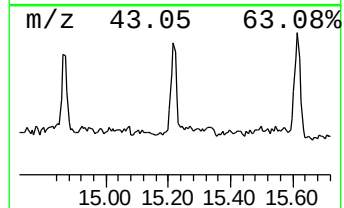
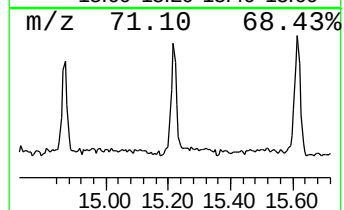
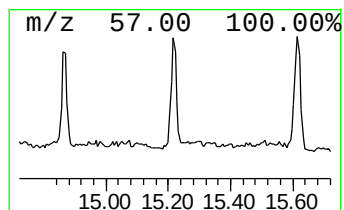
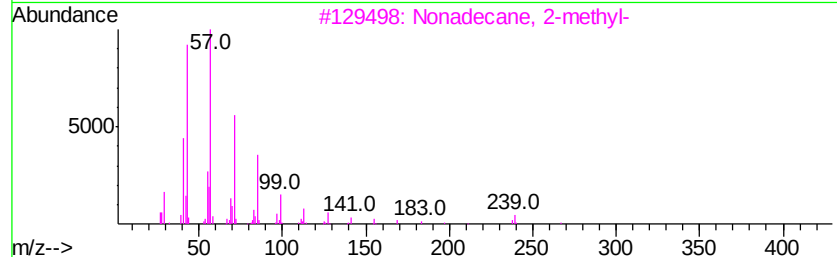
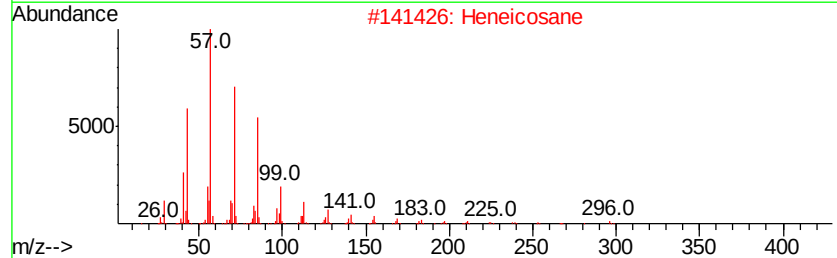
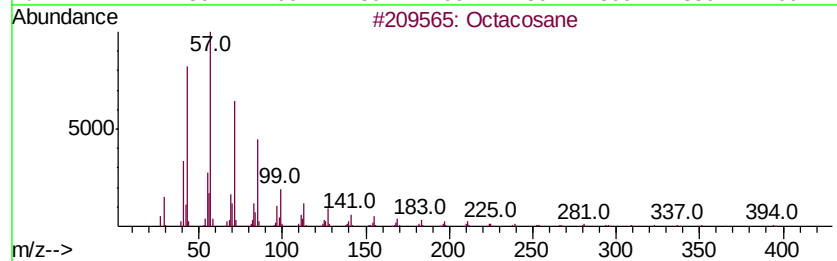
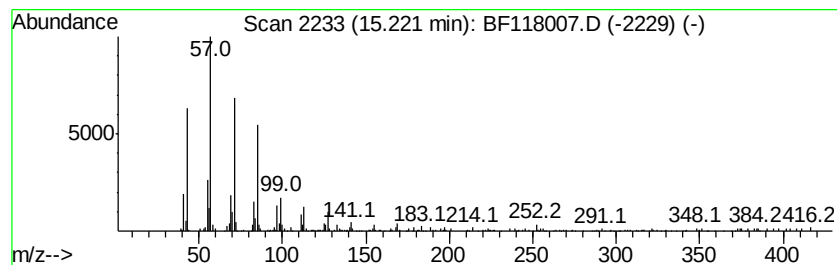
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.22	3.54 ng	198662	Perylene-d12		15.59
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Heneicosane	296	C21H44	000629-94-7	81
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	74
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
5	Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118007.D
Acq On : 26 Nov 2019 15:16
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Misc :
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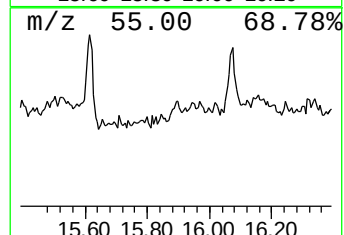
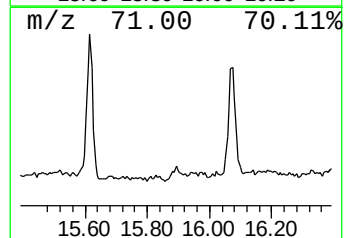
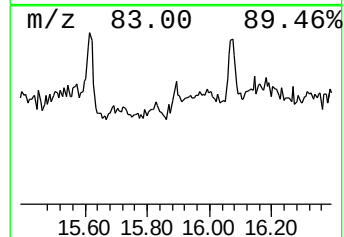
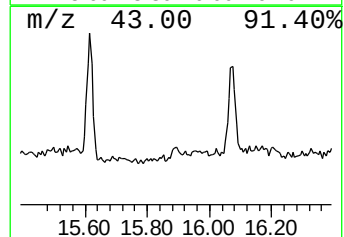
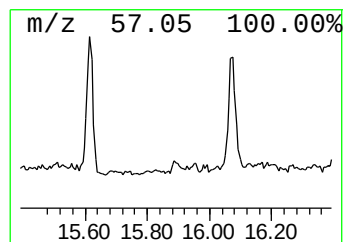
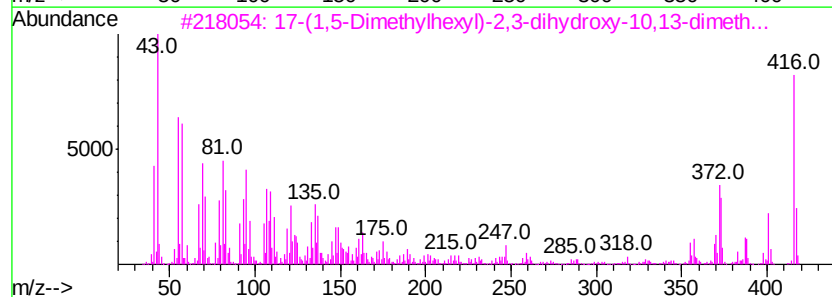
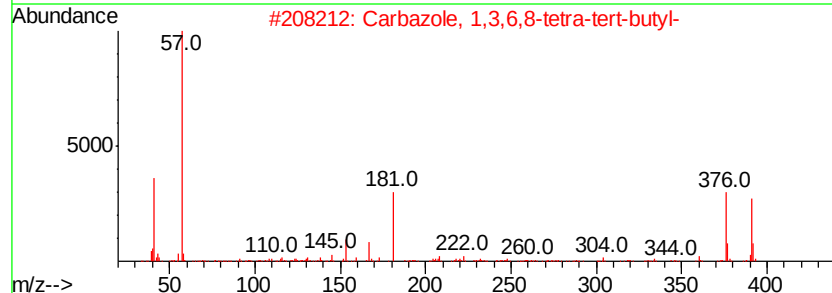
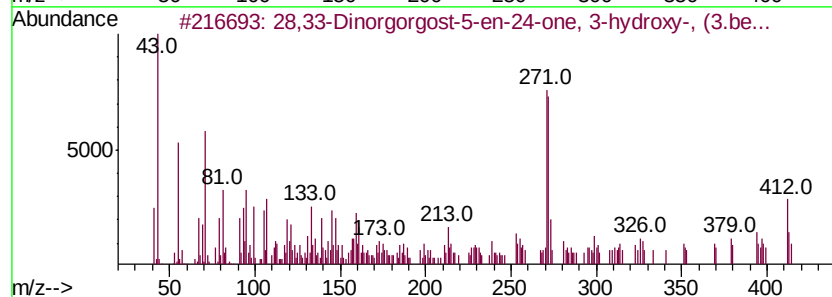
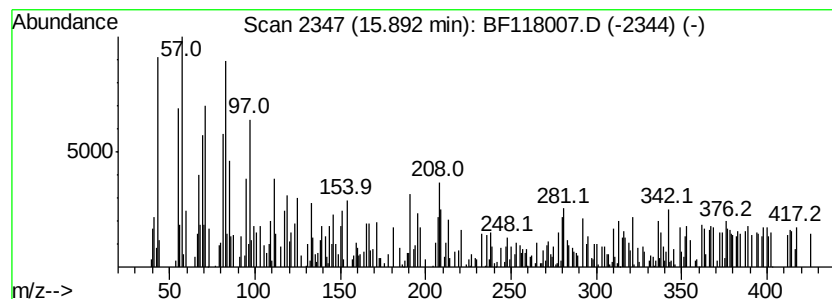
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown15.89 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.69 ng	151129	Perylene-d12	15.59

Hit#	of	3	Tentative ID	MW	MolForm	CAS#	Qual
1	28,33-Dinorgorgost-5-en-24-one, ...	412	C28H44O2	055064-61-4	11		
2	Carbazole, 1,3,6,8-tetra-tert-bu...	391	C28H41N	034601-54-2	10		
3	17-(1,5-Dimethylhexyl)-2,3-dihyd...	416	C27H44O3	1000210-26-4	7		



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ALS Vial : 10 Sample Multiplier: 1

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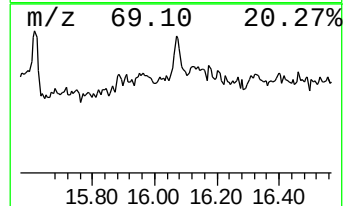
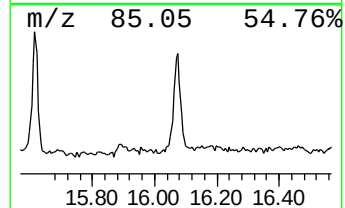
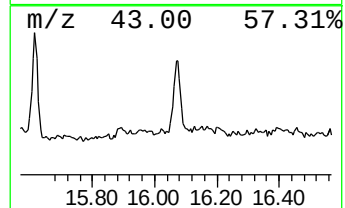
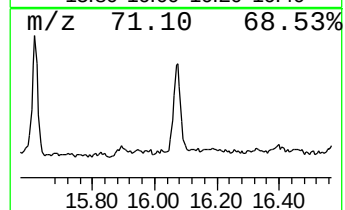
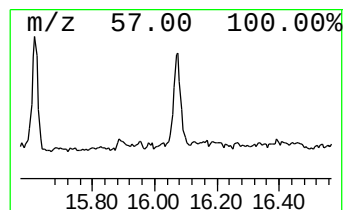
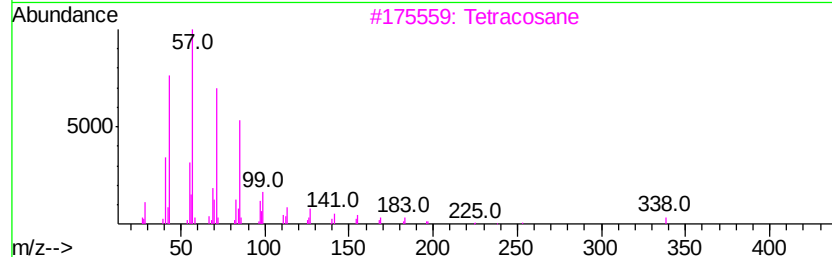
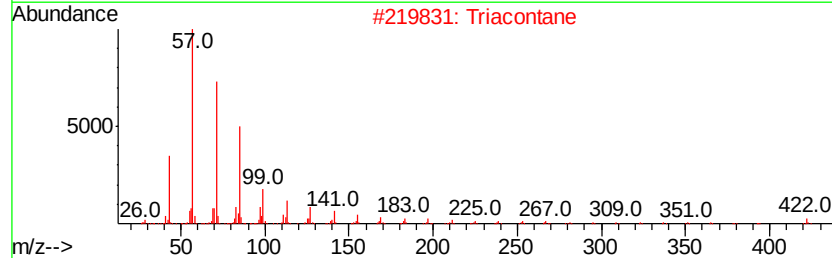
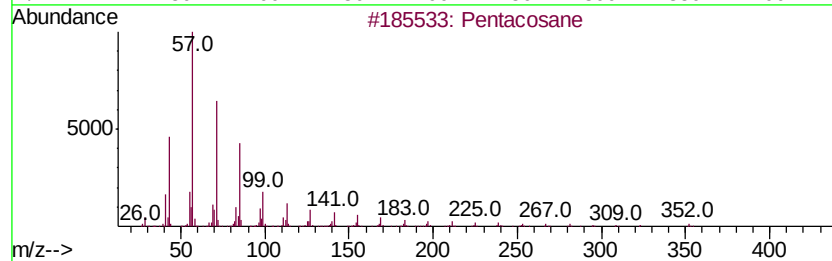
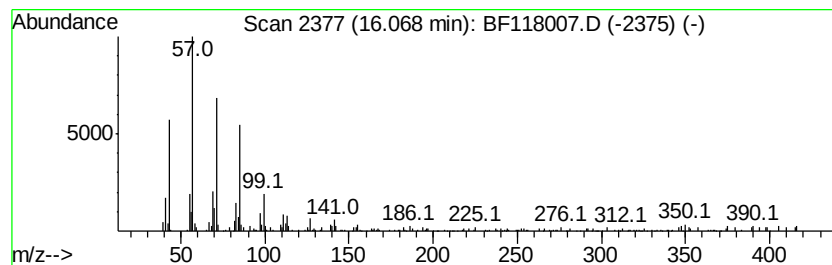
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.67 ng	149817	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	92
2		Triacotane	422	C30H62	000638-68-6	87
3		Tetracosane	338	C24H50	000646-31-1	83
4		2-methyloctacosane	408	C29H60	1000376-72-8	83
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112619\
 Data File : BF118007.D
 Acq On : 26 Nov 2019 15:16
 Operator : JU
 Sample : K5840-09 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-SE-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.14	11.0	ng	375233	1	6.89	684011	20.0
2-Pentanone, 4-hy...	5.09	5.4	ng	183173	1	6.89	684011	20.0
Xenon	6.66	31.0	ng	1061320	1	6.89	684011	20.0
n-Hexadecanoic acid	11.96	4.0	ng	183170	4	11.44	917394	20.0
Octadecane	13.25	2.3	ng	93432	5	14.09	812330	20.0
Eicosane	13.60	2.3	ng	91843	5	14.09	812330	20.0
Hexacosane	14.25	2.8	ng	113690	5	14.09	812330	20.0
Heptadecane, 9-oc...	14.55	2.6	ng	105895	5	14.09	812330	20.0
Heptadecane	14.87	2.7	ng	152453	6	15.59	1122760	20.0
Octacosane	15.22	3.5	ng	198662	6	15.59	1122760	20.0
unknown15.89	15.89	2.7	ng	151129	6	15.59	1122760	20.0
Pentacosane	16.07	2.7	ng	149817	6	15.59	1122760	20.0