

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
 Data File : BF118689.D
 Acq On : 24 Jan 2020 16:52
 Operator : CG/JU
 Sample : L1246-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3

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-BF012020.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	3	9	16	rVB	1288387	1726003	26.66%	3.172%
2	5.081	499	509	516	rVB2	73083	107984	1.67%	0.198%
3	5.481	572	577	581	rBV	4833031	5012154	77.41%	9.210%
4	6.487	743	748	758	rBV	4904600	5296048	81.80%	9.732%
5	6.863	808	812	815	rBV	1928865	1565055	24.17%	2.876%
6	7.022	835	839	842	rVB	5042346	4452986	68.78%	8.183%
7	7.422	902	907	910	rBV	3470566	3376229	52.15%	6.204%
8	8.145	1026	1030	1033	rBV	2243575	2026870	31.30%	3.725%
9	9.216	1208	1212	1216	rBV	6881271	6474618	100.00%	11.898%
10	9.334	1230	1232	1236	rVB	147270	128898	1.99%	0.237%
11	9.610	1275	1279	1282	rBV	1152450	993564	15.35%	1.826%
12	9.898	1324	1328	1331	rBV	2760940	2414280	37.29%	4.436%
13	10.680	1457	1461	1465	rBV	4433935	4111795	63.51%	7.556%
14	11.380	1575	1580	1583	rBV	2681110	2362163	36.48%	4.341%
15	11.604	1614	1618	1622	rBV	79703	78400	1.21%	0.144%
16	11.904	1666	1669	1673	rBV2	517841	402825	6.22%	0.740%
17	12.116	1702	1705	1710	rVB3	67357	78818	1.22%	0.145%
18	12.422	1752	1757	1761	rBV4	168158	196593	3.04%	0.361%
19	12.469	1761	1765	1768	rBV3	69126	75138	1.16%	0.138%
20	12.586	1783	1785	1788	rBV	114755	97839	1.51%	0.180%
21	12.616	1788	1790	1795	rVB3	47826	70338	1.09%	0.129%
22	12.686	1799	1802	1809	rVB2	368327	341968	5.28%	0.628%
23	12.792	1816	1820	1821	rBV2	152406	145200	2.24%	0.267%
24	12.816	1821	1824	1826	rVV2	174311	179817	2.78%	0.330%
25	12.839	1826	1828	1831	rVB	86810	71175	1.10%	0.131%
26	12.963	1844	1849	1852	rBV	6603140	5973291	92.26%	10.976%
27	13.198	1886	1889	1895	rVB2	93887	88962	1.37%	0.163%
28	13.857	1997	2001	2010	rVB2	291941	397883	6.15%	0.731%
29	14.010	2022	2027	2030	rBV	1927176	1799225	27.79%	3.306%
30	14.180	2052	2056	2062	rVB	185621	174744	2.70%	0.321%
31	14.486	2104	2108	2112	rBV	323075	288873	4.46%	0.531%
32	14.792	2156	2160	2168	rBV	318085	362811	5.60%	0.667%
33	14.868	2169	2173	2181	rVV	188234	198269	3.06%	0.364%
34	15.045	2199	2203	2206	rBV	46405	77201	1.19%	0.142%

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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 >
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35	15.127	2213	2217	2227	rBV	371599	456029	7.04%	0.838%
36	15.474	2270	2276	2279	rBV	1394870	1715647	26.50%	3.153%
37	15.510	2279	2282	2289	rVB	301423	392924	6.07%	0.722%
38	15.945	2351	2356	2362	rBV	227699	348351	5.38%	0.640%
39	16.457	2436	2443	2449	rBV	124541	261457	4.04%	0.480%
40	17.051	2538	2544	2550	rBV3	47843	96938	1.50%	0.178%

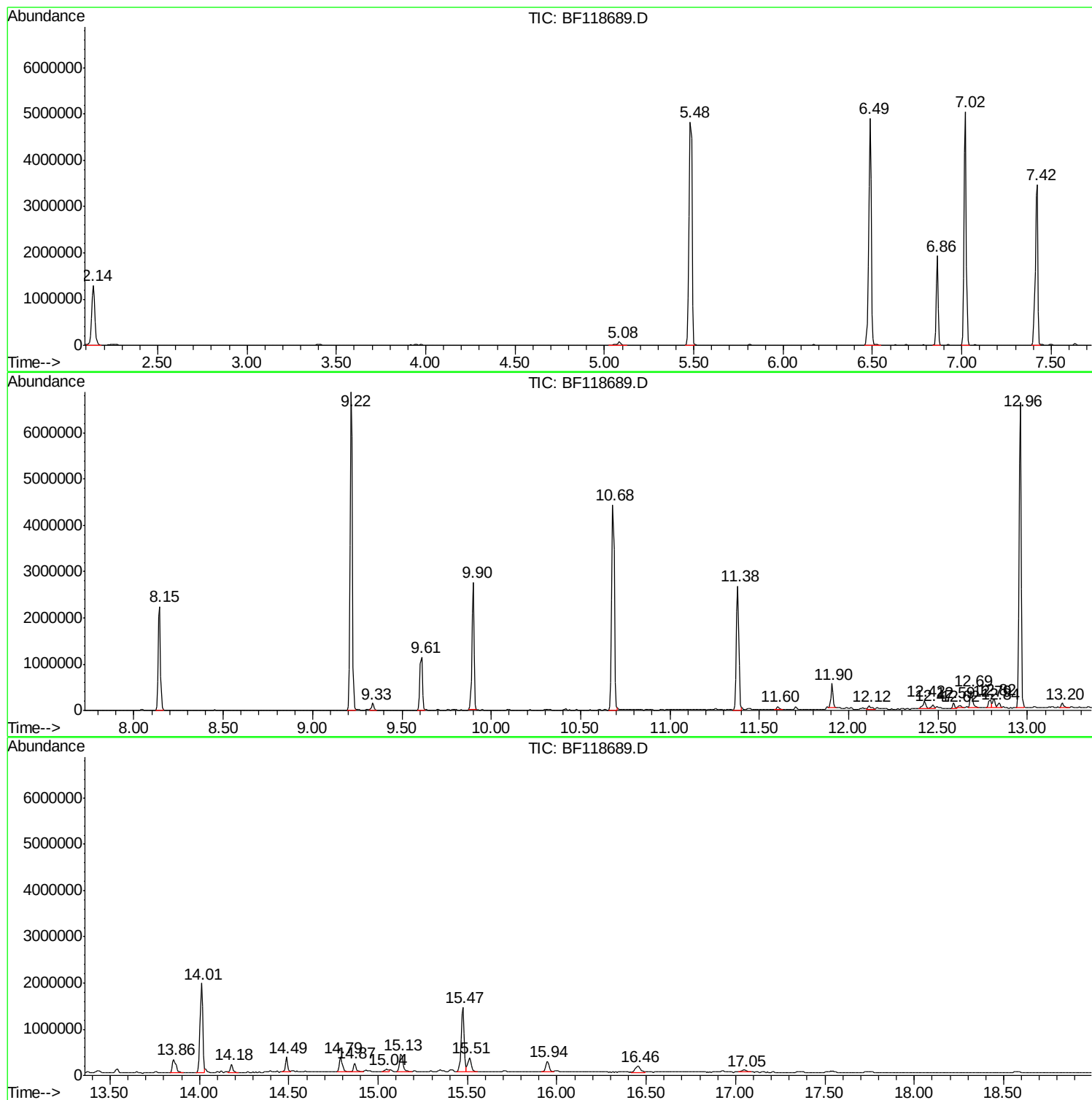
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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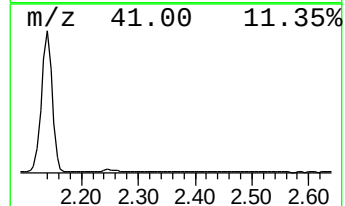
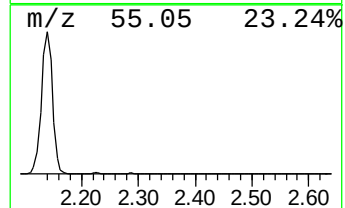
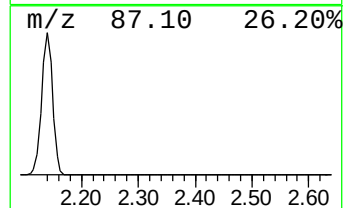
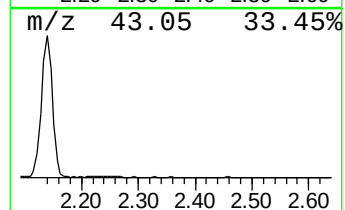
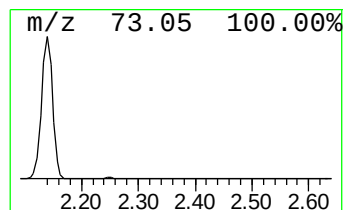
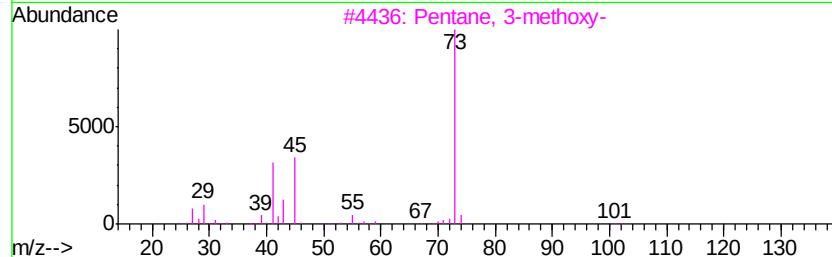
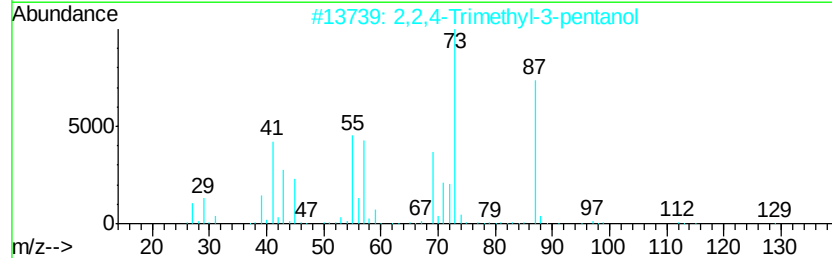
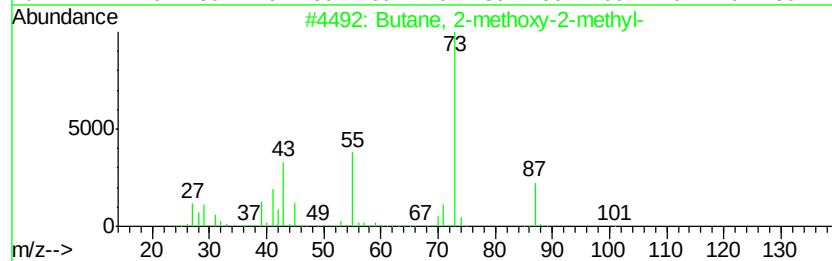
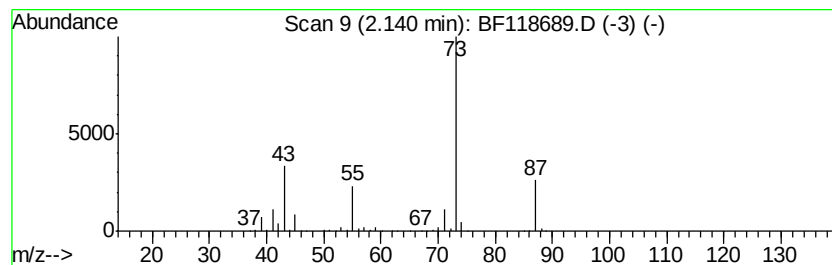
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	22.06 ng	1726000	1,4-Dichlorobenzene-d4	6.86

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	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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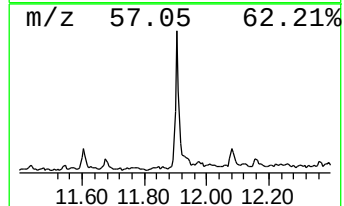
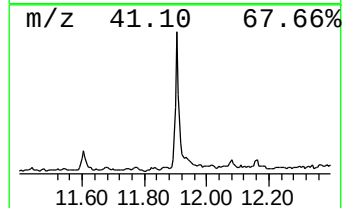
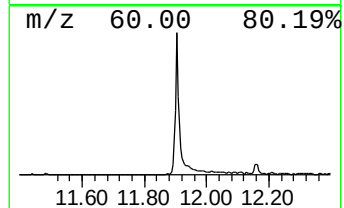
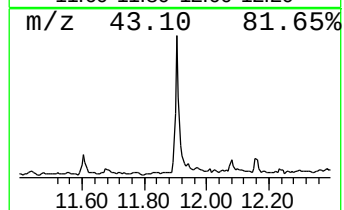
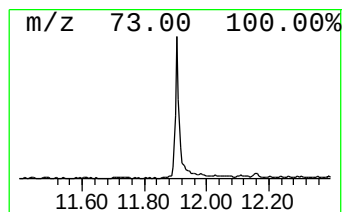
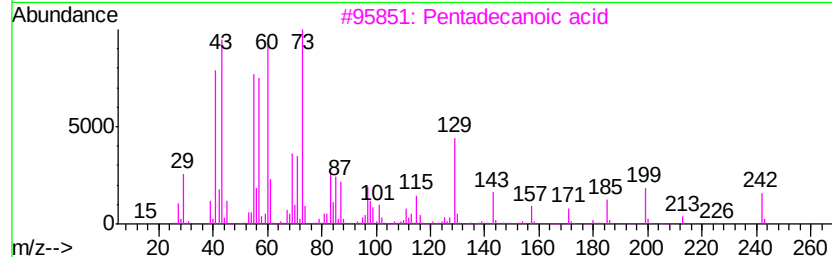
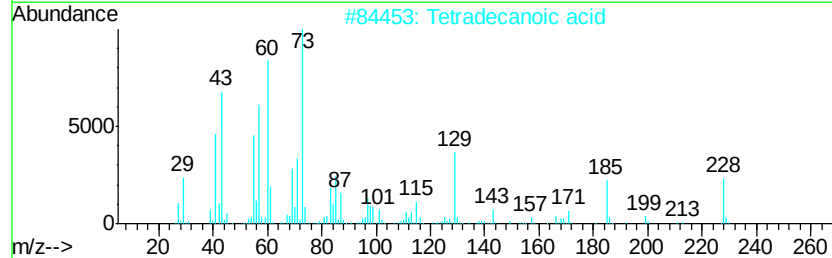
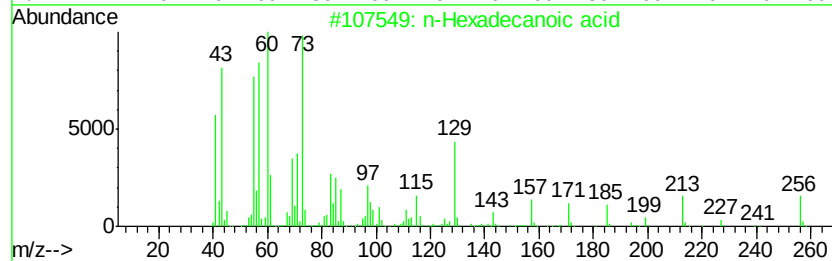
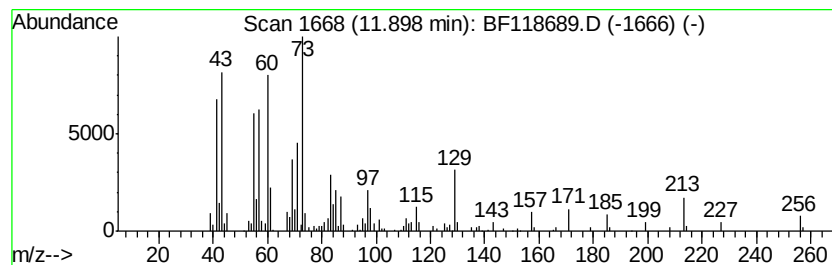
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.41 ng	402825	Phenanthrene-d10	11.38

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	62



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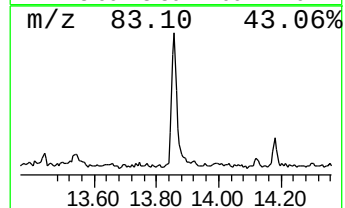
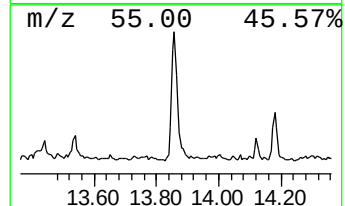
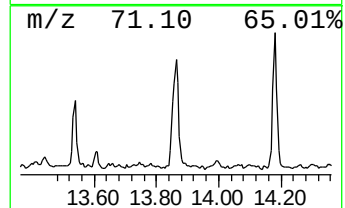
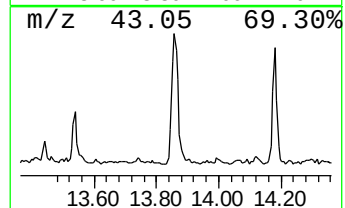
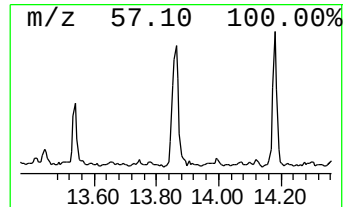
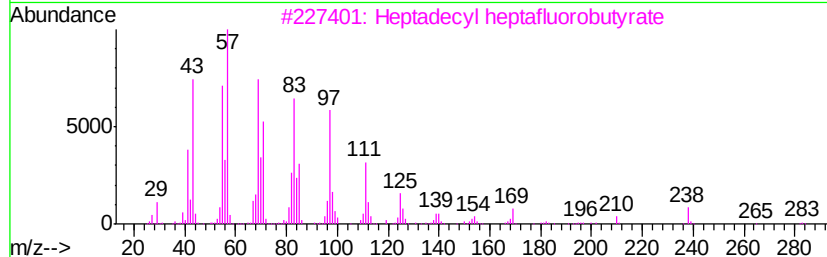
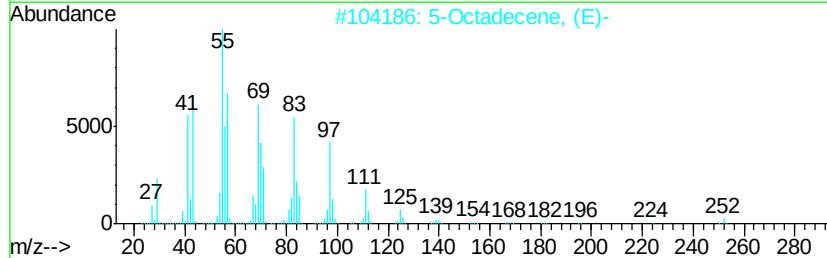
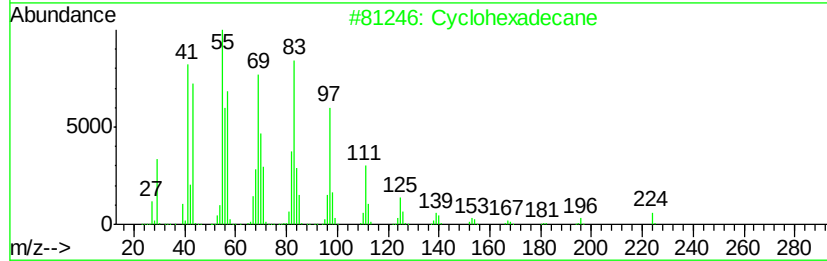
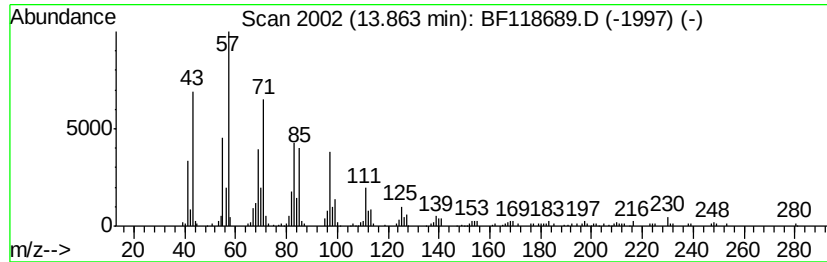
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	4.42 ng	397883	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
3	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93



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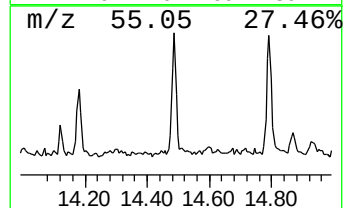
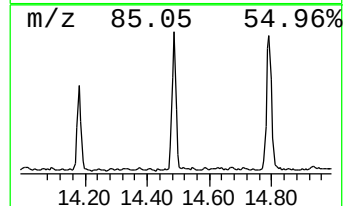
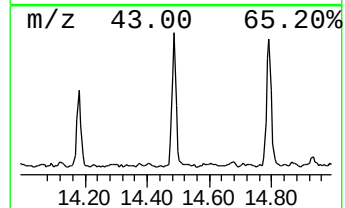
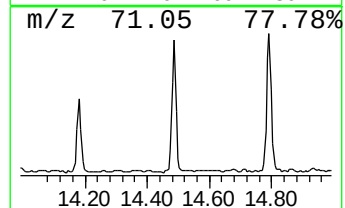
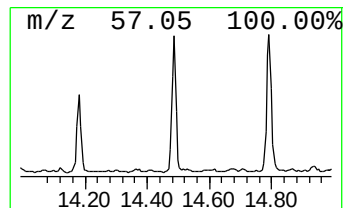
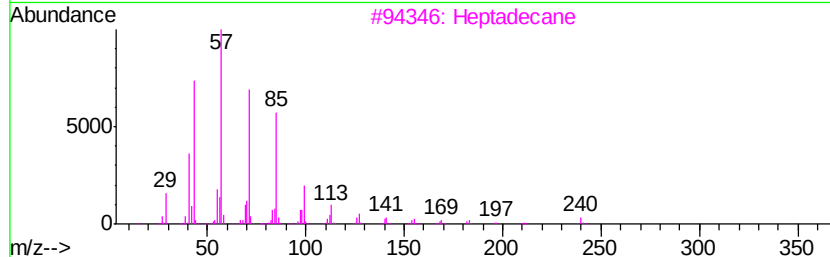
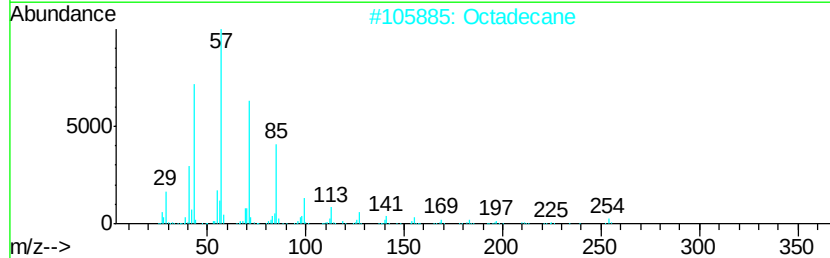
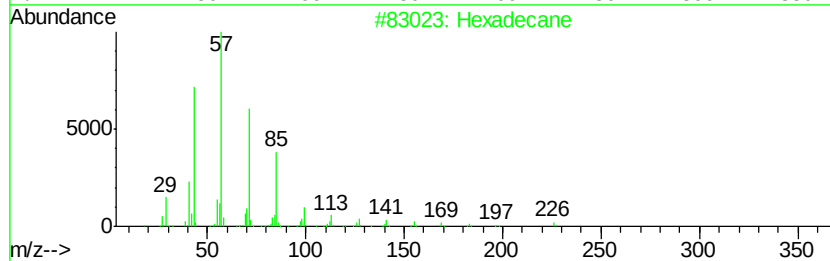
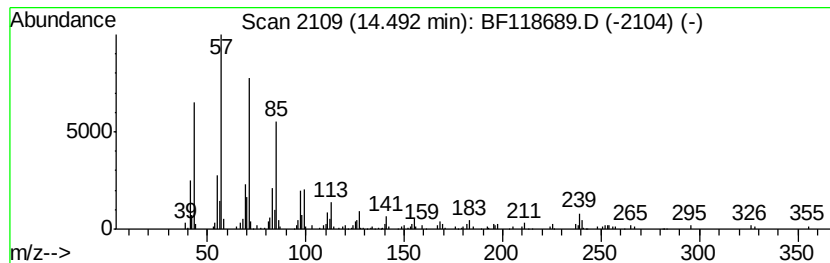
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	3.21 ng	288873	Chrysene-d12	14.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	96
2	Octadecane	254 C18H38	000593-45-3	95
3	Heptadecane	240 C17H36	000629-78-7	95
4	Tetracosane	338 C24H50	000646-31-1	91
5	Heneicosane	296 C21H44	000629-94-7	91



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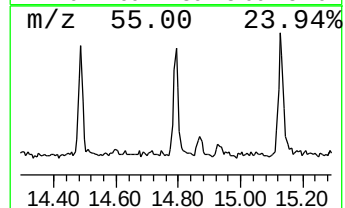
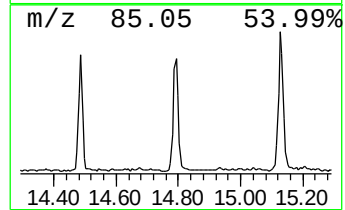
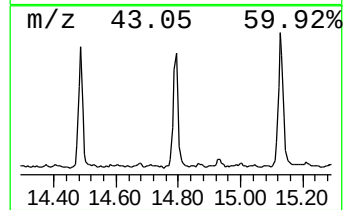
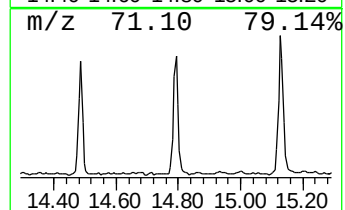
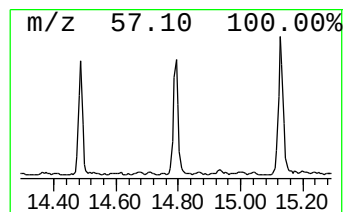
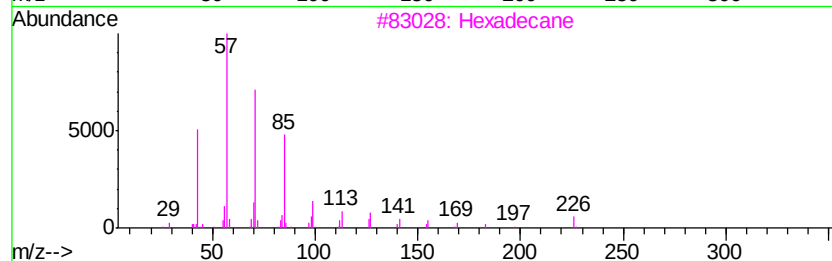
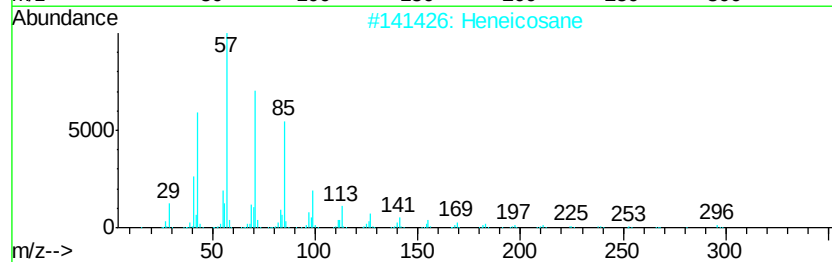
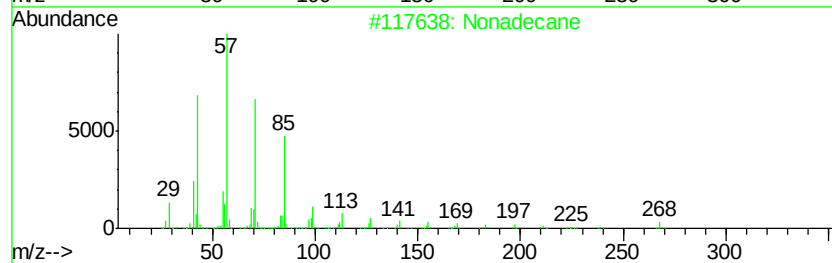
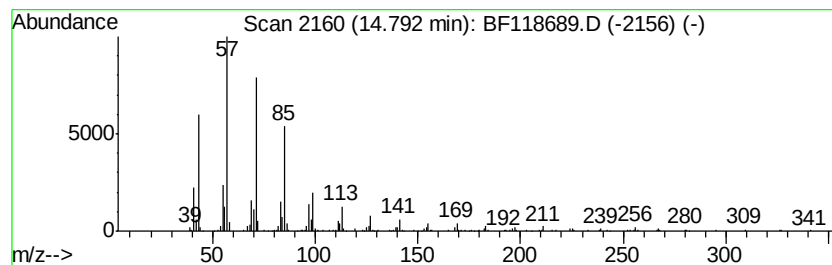
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.23 ng	362811	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	Heneicosane		296	C21H44	000629-94-7	91
3	Hexadecane		226	C16H34	000544-76-3	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Tetracosane		338	C24H50	000646-31-1	91



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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

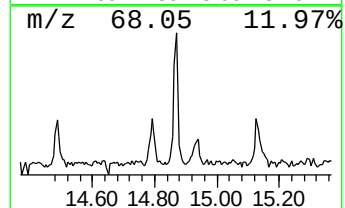
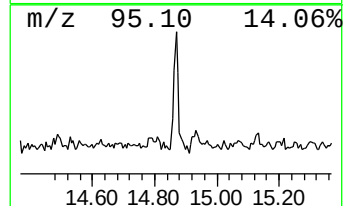
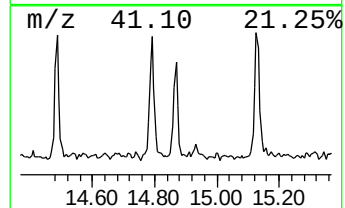
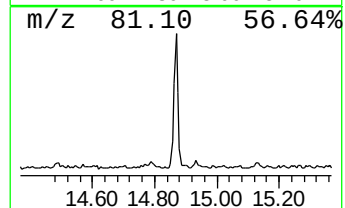
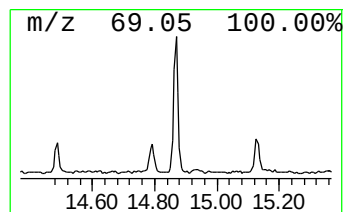
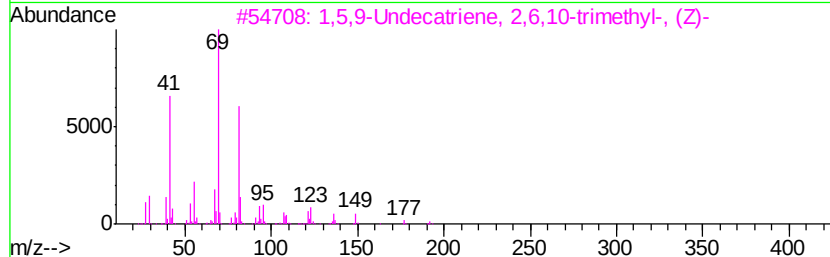
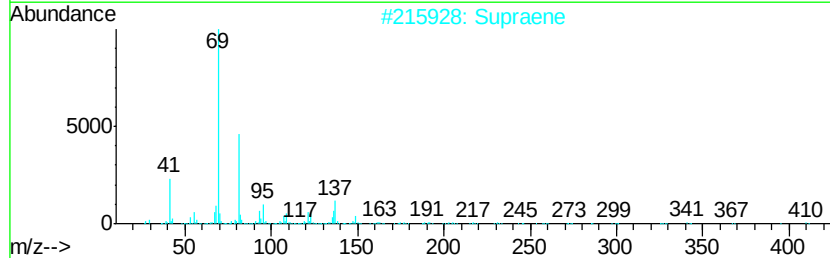
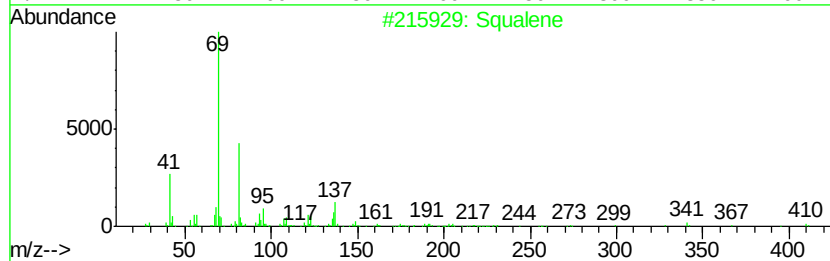
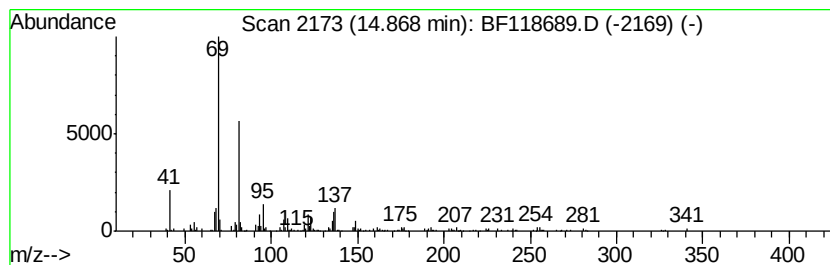
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.31 ng	198269	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	87
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5		trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
Data File : BF118689.D
Acq On : 24 Jan 2020 16:52
Operator : CG/JU
Sample : L1246-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

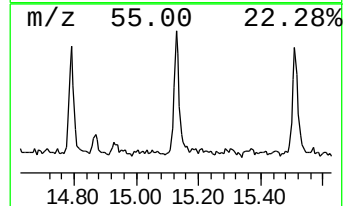
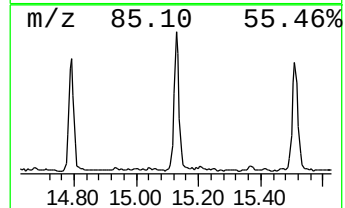
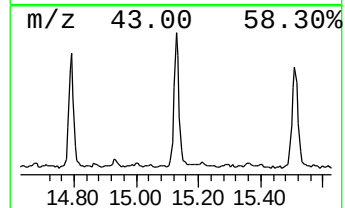
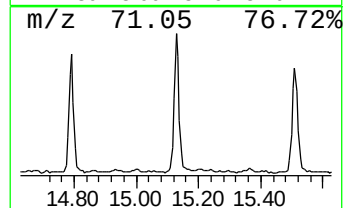
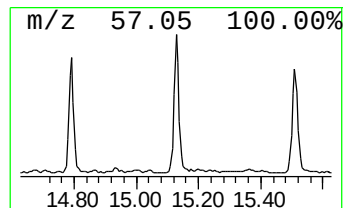
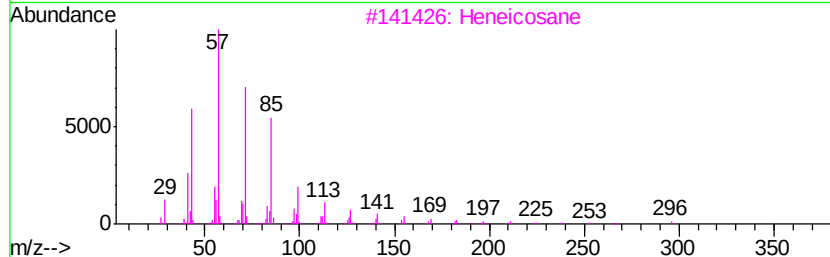
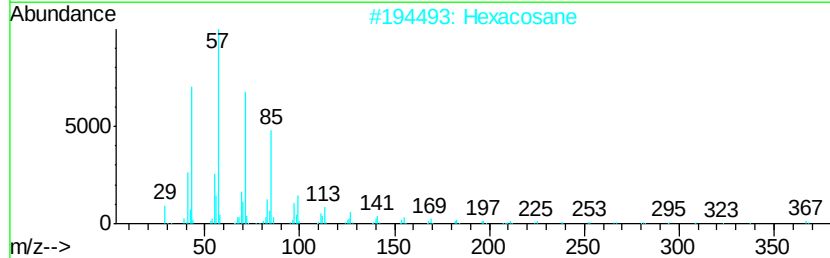
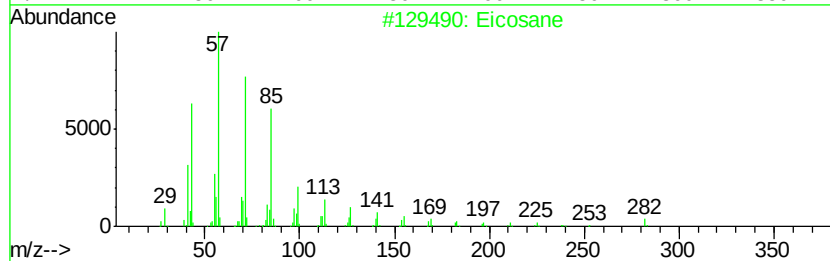
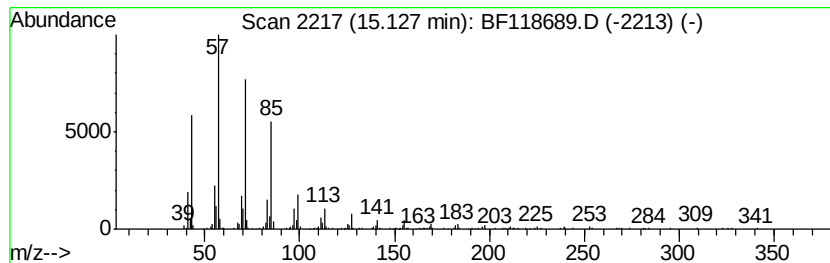
Instrument :
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ClientSampleId :
SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	5.32 ng	456029	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Hexacosane	366 C26H54	000630-01-3	94
3	Heneicosane	296 C21H44	000629-94-7	91
4	2-methyloctacosane	408 C29H60	1000376-72-8	91
5	Tetracosane	338 C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
Data File : BF118689.D
Acq On : 24 Jan 2020 16:52
Operator : CG/JU
Sample : L1246-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

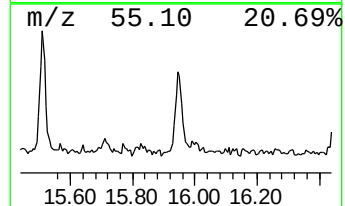
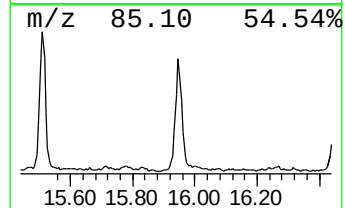
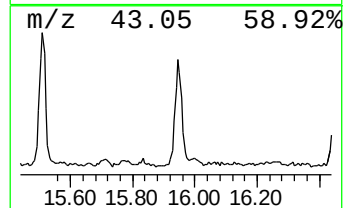
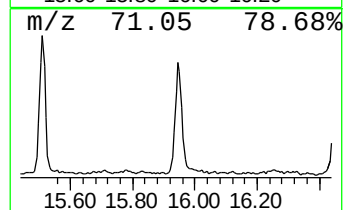
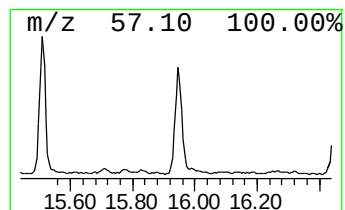
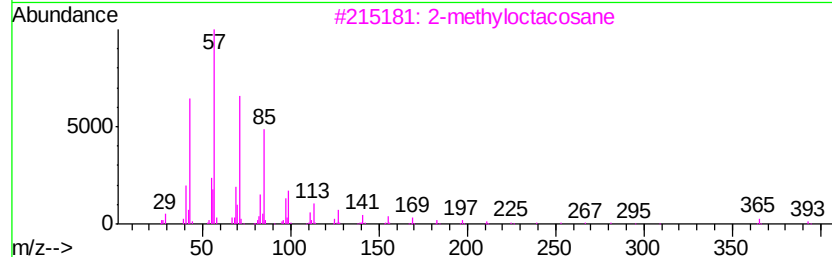
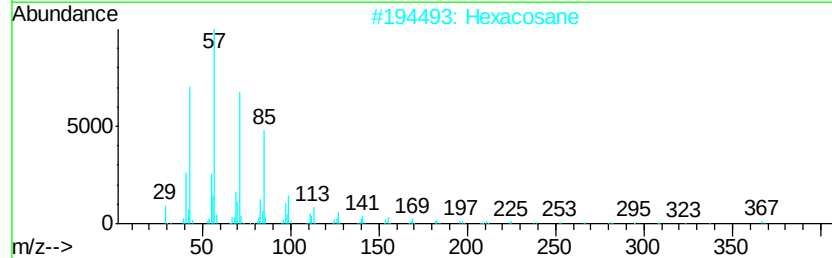
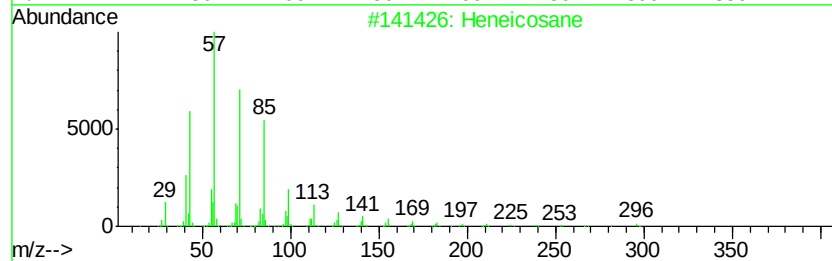
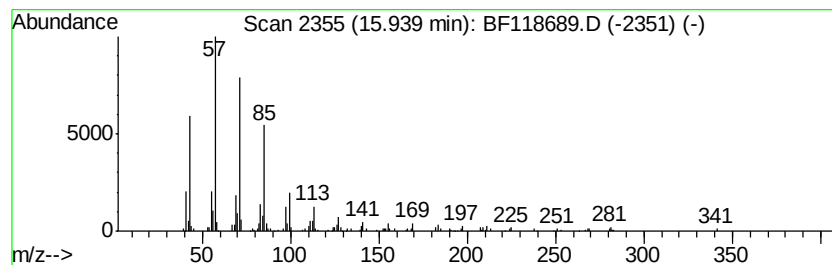
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.06 ng	348351	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012420\
Data File : BF118689.D
Acq On : 24 Jan 2020 16:52
Operator : CG/JU
Sample : L1246-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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	22.1	ng	1726000	1	6.86	1565060	20.0
n-Hexadecanoic acid	11.90	3.4	ng	402825	4	11.38	2362160	20.0
Cyclohexadecane	13.86	4.4	ng	397883	5	14.01	1799230	20.0
Hexadecane	14.49	3.2	ng	288873	5	14.01	1799230	20.0
Nonadecane	14.79	4.2	ng	362811	6	15.47	1715650	20.0
Squalene	14.87	2.3	ng	198269	6	15.47	1715650	20.0
Hexacosane	15.13	5.3	ng	456029	6	15.47	1715650	20.0
2-methyloctacosane	15.94	4.1	ng	348351	6	15.47	1715650	20.0