

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021119\
 Data File : BF112479.D
 Acq On : 11 Feb 2019 14:34
 Operator : JU/SJ
 Sample : K1452-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEST-PIT-2

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-BF012519.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	2.134	3	8	15	rVB	164355	216165	4.10%	0.447%
2	5.069	504	507	519	rBV	122390	201050	3.81%	0.416%
3	5.475	572	576	605	rBV	3946818	4103158	77.76%	8.485%
4	6.486	743	748	751	rBV	3883683	4239651	80.35%	8.767%
5	6.610	765	769	773	rBV	4573690	4614586	87.45%	9.542%
6	6.833	803	807	813	rBV	955018	916599	17.37%	1.895%
7	6.986	829	833	837	rBV	3496405	3479455	65.94%	7.195%
8	7.398	898	903	906	rBV	2721475	2780040	52.69%	5.749%
9	8.110	1020	1024	1038	rBV	1186837	1232408	23.36%	2.548%
10	9.186	1202	1207	1218	rBV	4983602	5276560	100.00%	10.911%
11	9.580	1271	1274	1279	rBV	337788	291669	5.53%	0.603%
12	9.869	1318	1323	1336	rVB	1627206	1510166	28.62%	3.123%
13	10.663	1454	1458	1470	rBV	3657822	3974123	75.32%	8.218%
14	11.357	1572	1576	1579	rBV	1801073	1602482	30.37%	3.314%
15	11.380	1579	1580	1587	rVB	202887	138024	2.62%	0.285%
16	11.880	1662	1665	1673	rVB3	484032	542944	10.29%	1.123%
17	11.968	1677	1680	1683	rVV2	123572	138324	2.62%	0.286%
18	11.992	1683	1684	1690	rVB	79887	63611	1.21%	0.132%
19	12.151	1708	1711	1715	rBV3	55883	58242	1.10%	0.120%
20	12.192	1715	1718	1721	rVB2	62865	65725	1.25%	0.136%
21	12.410	1752	1755	1757	rBV	104591	93976	1.78%	0.194%
22	12.445	1757	1761	1763	rVB3	41326	62540	1.19%	0.129%
23	12.574	1780	1783	1786	rBV	252587	241575	4.58%	0.500%
24	12.663	1795	1798	1805	rBV2	432035	427575	8.10%	0.884%
25	12.804	1816	1822	1824	rBV	330829	338109	6.41%	0.699%
26	12.945	1840	1846	1849	rBV	5066926	5226687	99.05%	10.808%
27	13.157	1880	1882	1887	rVB3	77273	81067	1.54%	0.168%
28	13.233	1893	1895	1899	rVB2	64423	70139	1.33%	0.145%
29	13.362	1914	1917	1920	rBV	50742	54794	1.04%	0.113%
30	13.498	1938	1940	1943	rBV	68058	56842	1.08%	0.118%
31	13.827	1992	1996	2004	rBV	617037	790379	14.98%	1.634%
32	14.004	2021	2026	2029	rBV	1284674	1403688	26.60%	2.903%
33	14.027	2029	2030	2033	rVB	164317	95076	1.80%	0.197%
34	14.145	2047	2050	2052	rBV	163513	139897	2.65%	0.289%

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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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35	14.392	2087	2092	2096	rBV	60436	95996	1.82%	0.199%
36	14.445	2099	2101	2104	rBV	189054	179236	3.40%	0.371%
37	14.751	2149	2153	2156	rVB	287836	286867	5.44%	0.593%
38	14.821	2162	2165	2169	rVB	104726	117636	2.23%	0.243%
39	15.051	2200	2204	2206	rBV	93011	135434	2.57%	0.280%
40	15.086	2206	2210	2214	rVB2	336930	432477	8.20%	0.894%
41	15.351	2252	2255	2258	rVB	60290	70984	1.35%	0.147%
42	15.415	2262	2266	2268	rBV	71344	92025	1.74%	0.190%
43	15.468	2268	2275	2289	rVB2	820696	1515000	28.71%	3.133%
44	15.886	2341	2346	2352	rVB	250126	362587	6.87%	0.750%
45	15.956	2354	2358	2364	rVB9	35399	71117	1.35%	0.147%
46	16.380	2425	2430	2441	rVB3	149705	291279	5.52%	0.602%
47	16.962	2524	2529	2537	rVB3	89135	180411	3.42%	0.373%

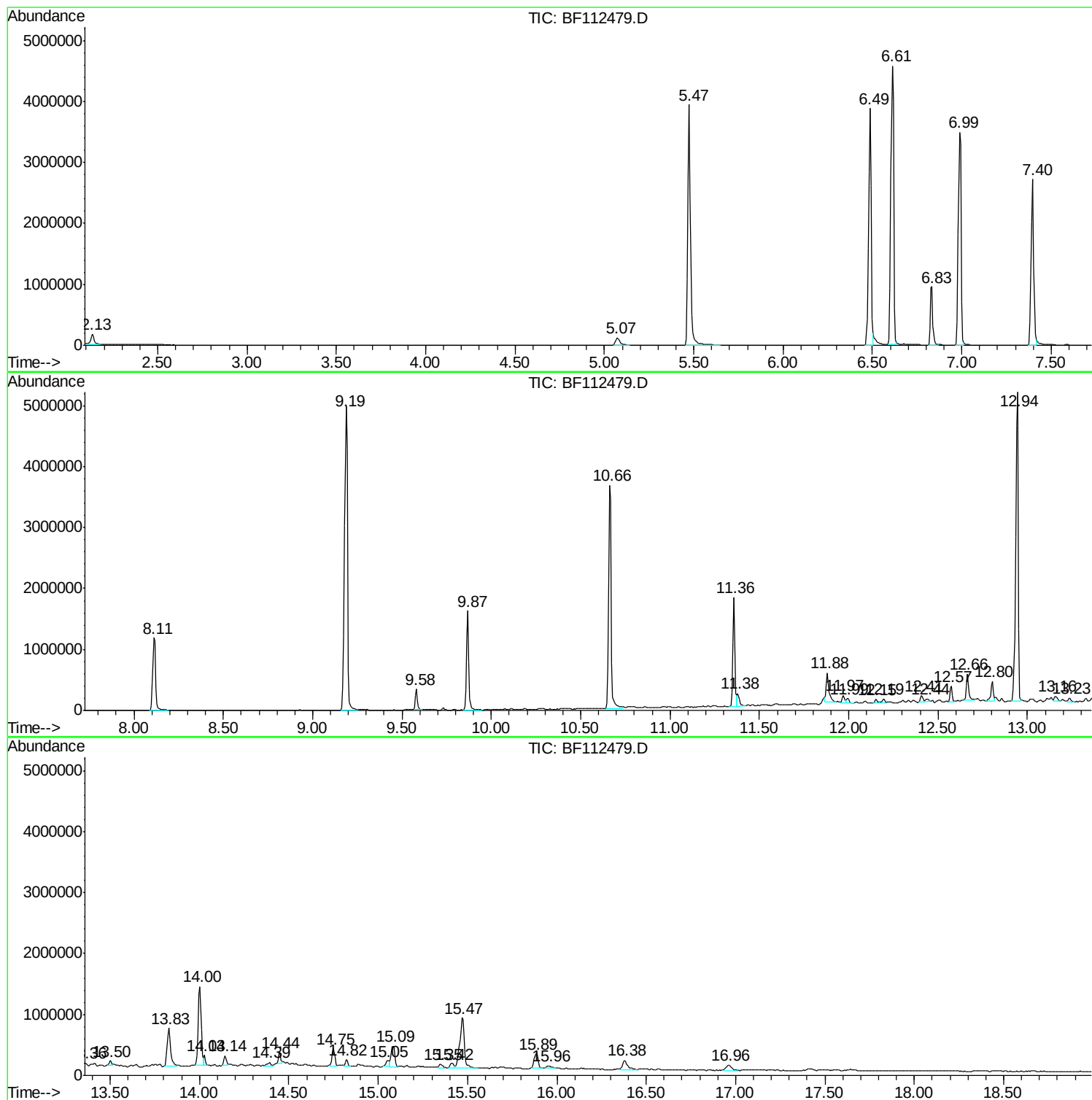
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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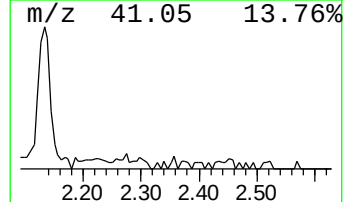
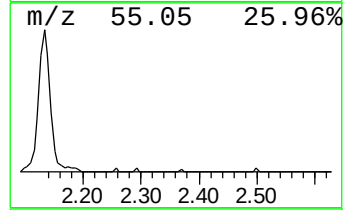
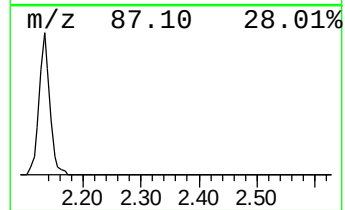
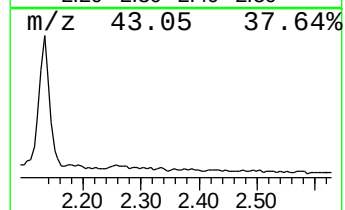
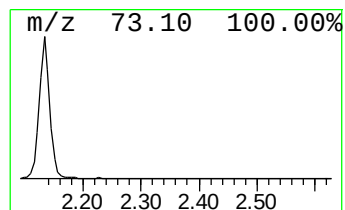
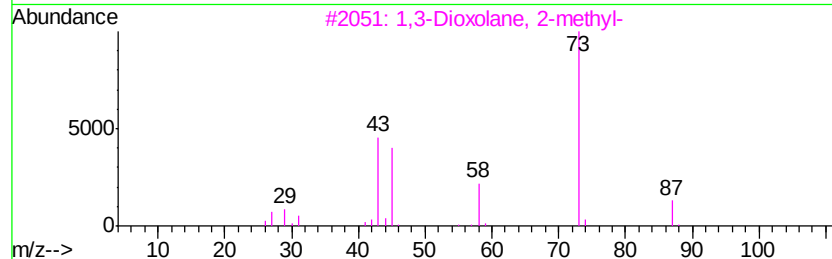
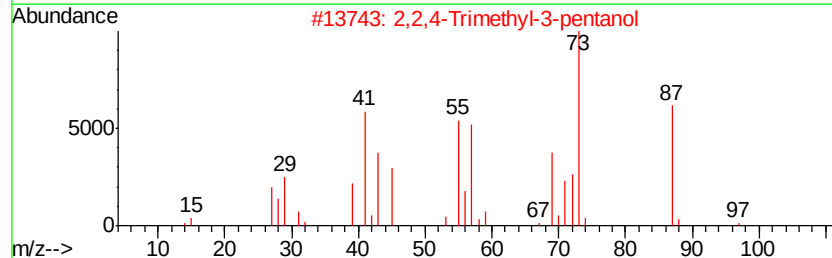
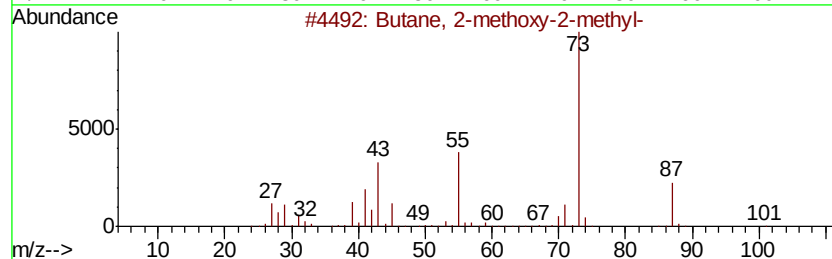
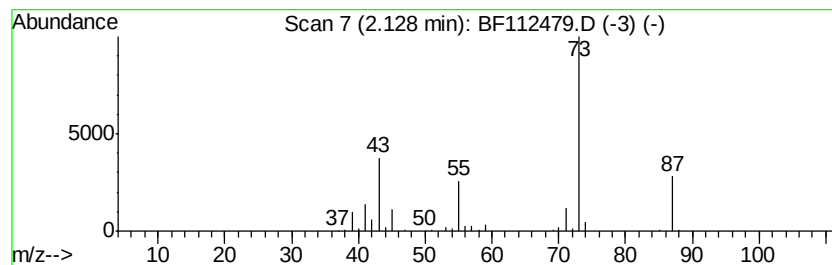
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	4.72 ng	216165	1,4-Dichlorobenzene-d4	6.83

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	37
4		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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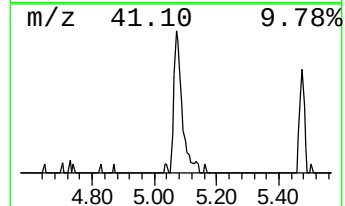
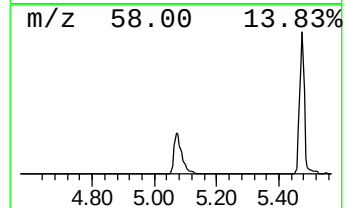
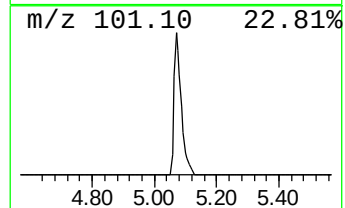
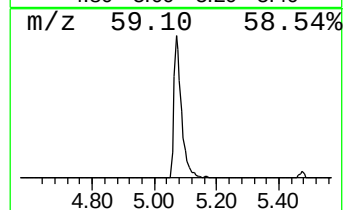
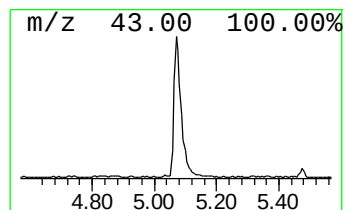
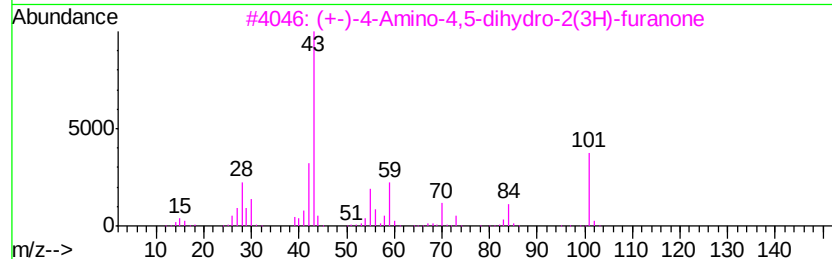
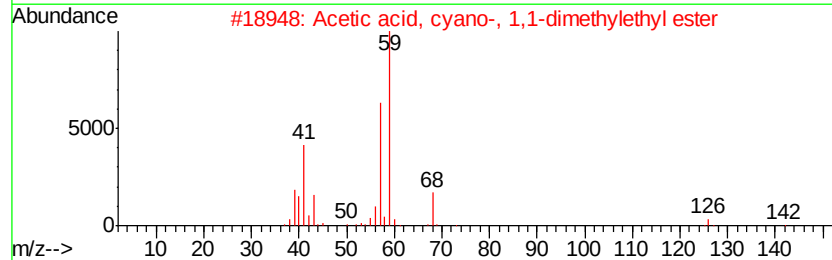
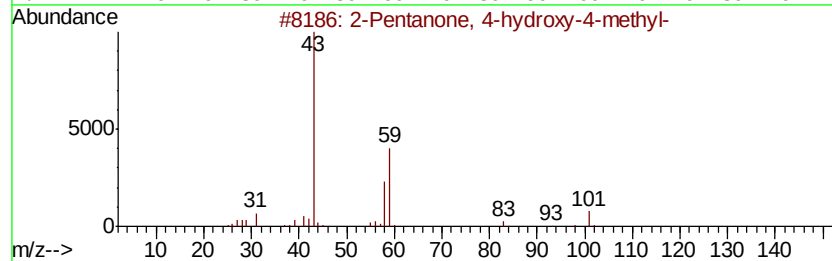
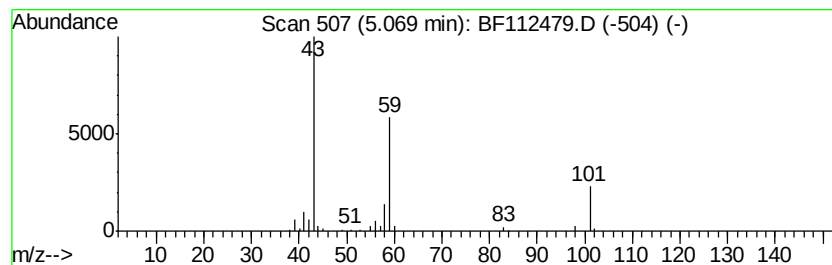
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	4.39 ng	201050	1,4-Dichlorobenzene-d4	6.83

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	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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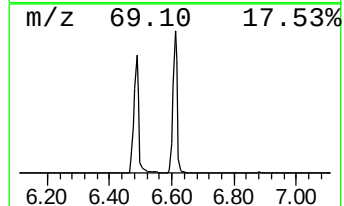
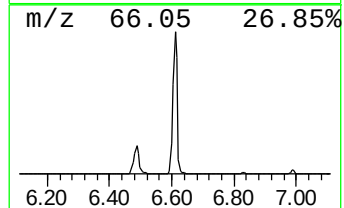
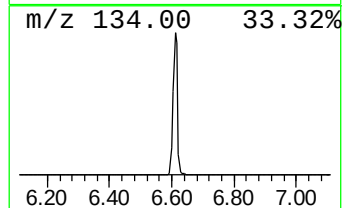
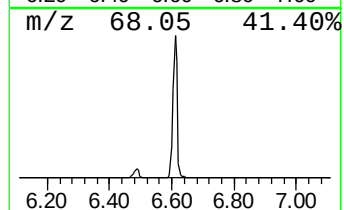
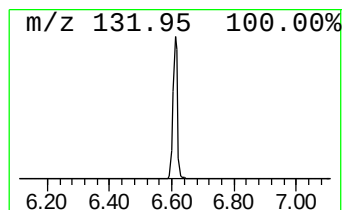
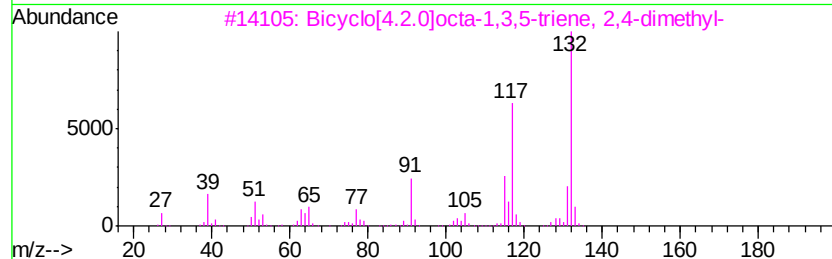
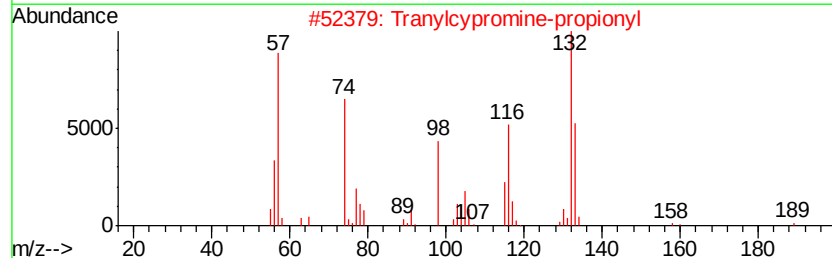
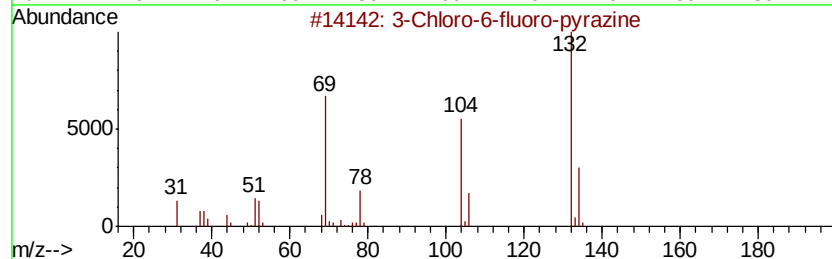
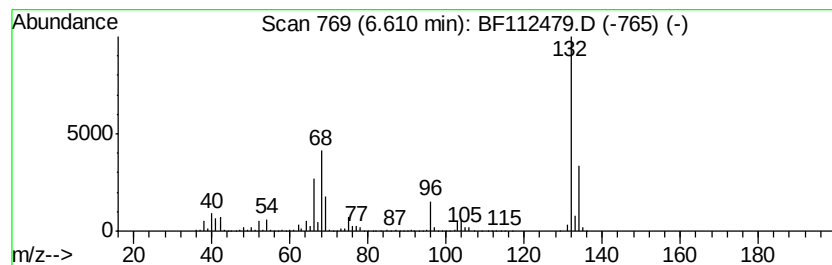
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	100.69 ng	4614590	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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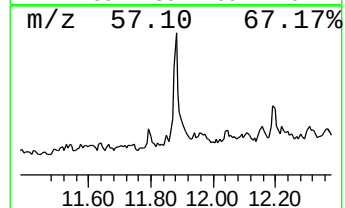
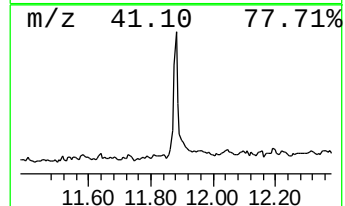
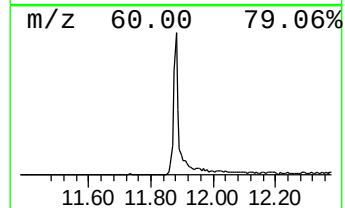
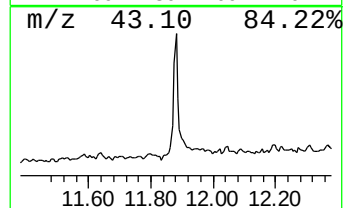
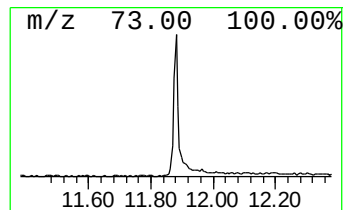
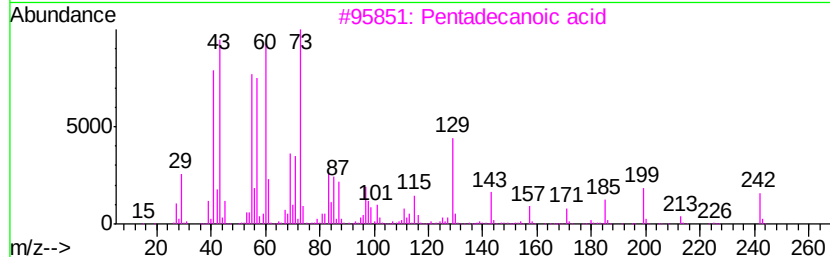
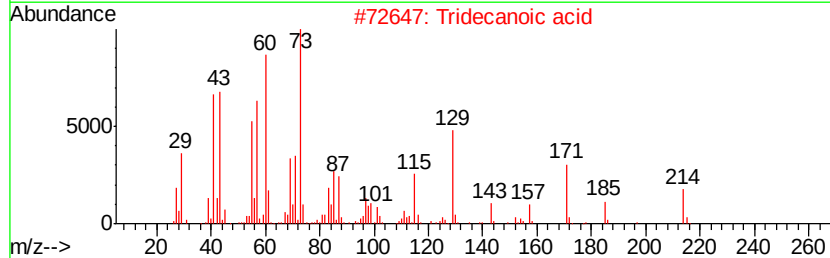
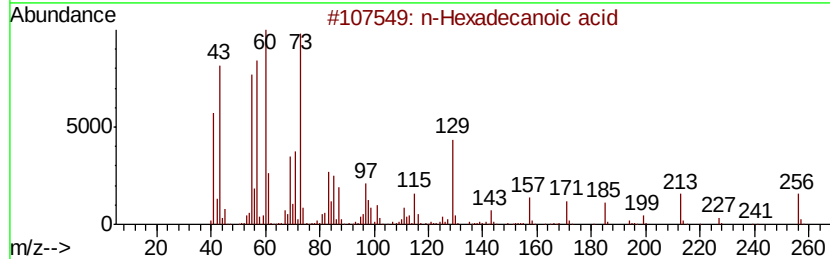
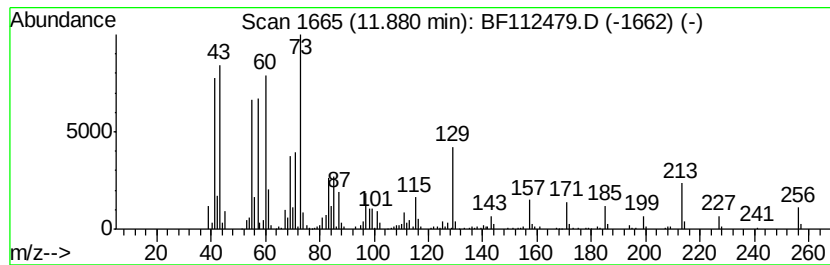
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	6.78 ng	542944	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		Undecanoic acid	186	C11H22O2	000112-37-8	74



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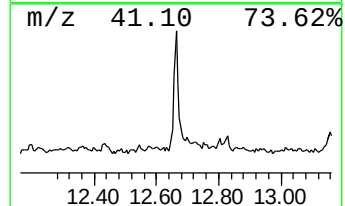
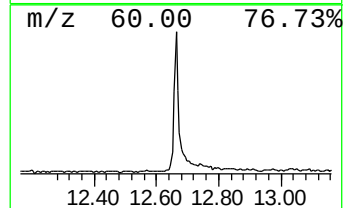
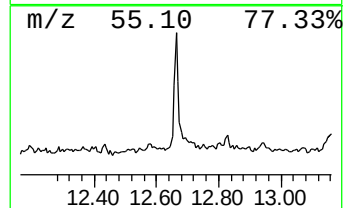
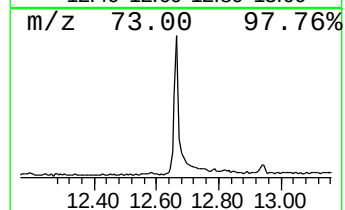
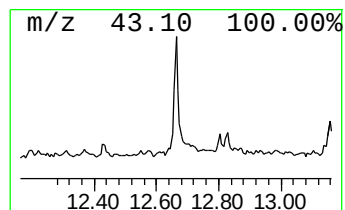
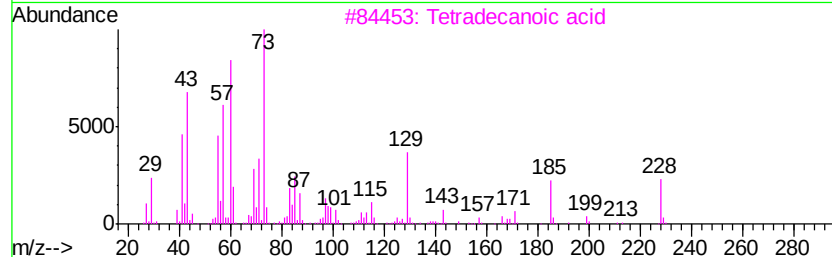
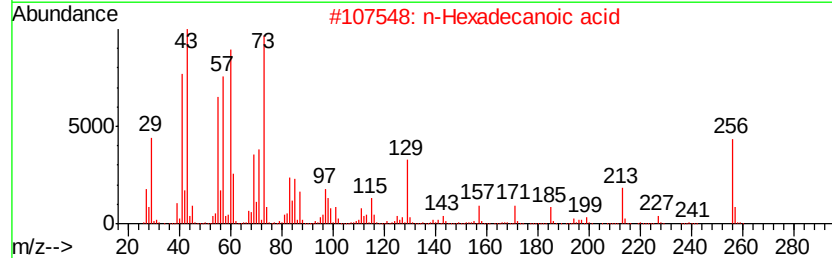
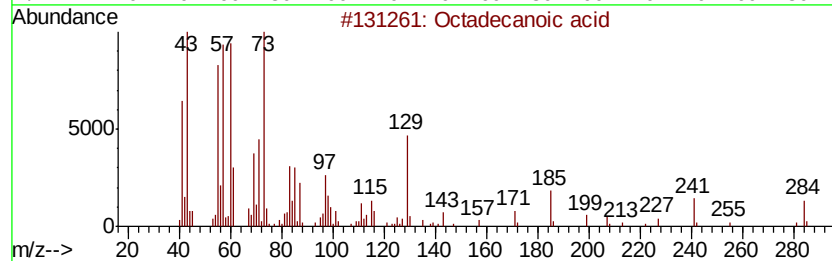
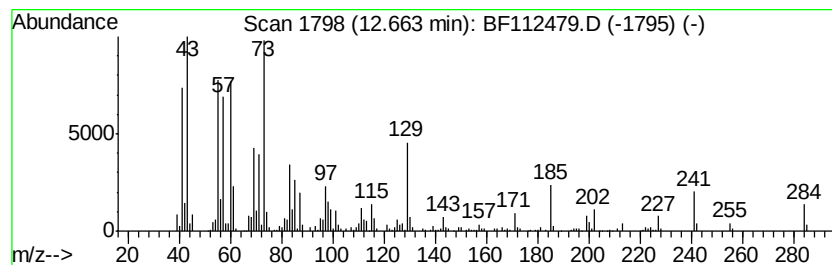
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	5.34 ng	427575	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
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Acq On : 11 Feb 2019 14:34
Operator : JU/SJ
Sample : K1452-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

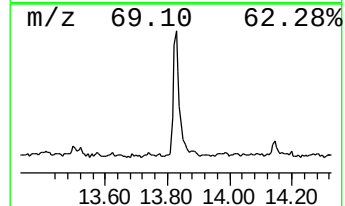
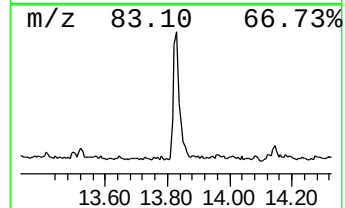
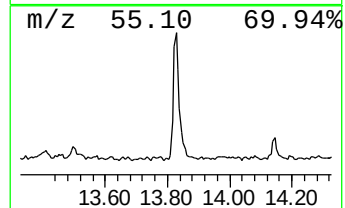
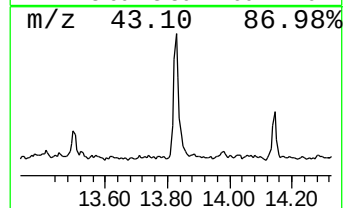
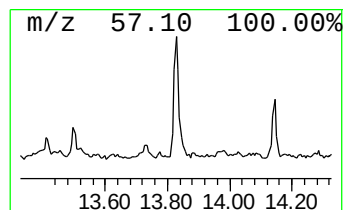
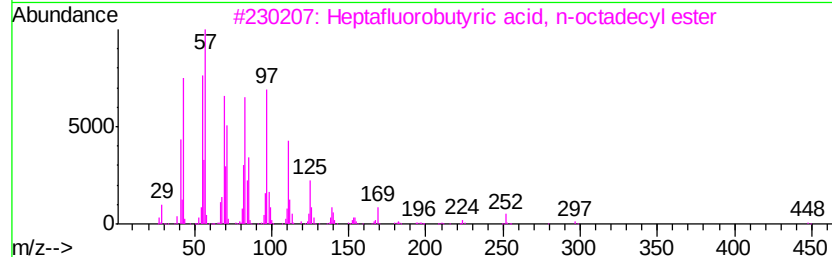
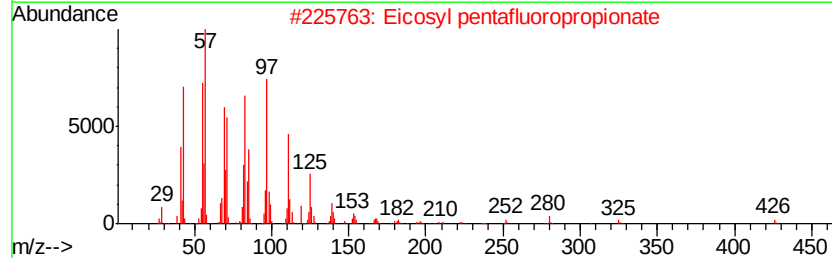
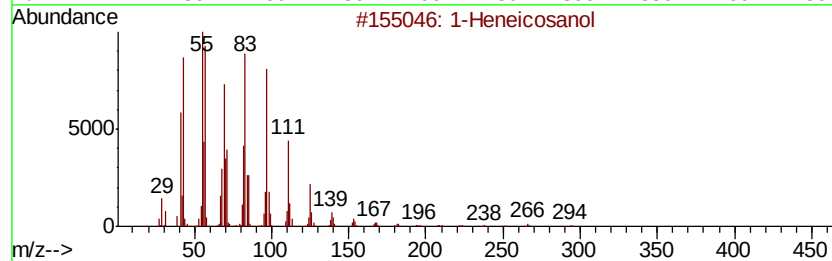
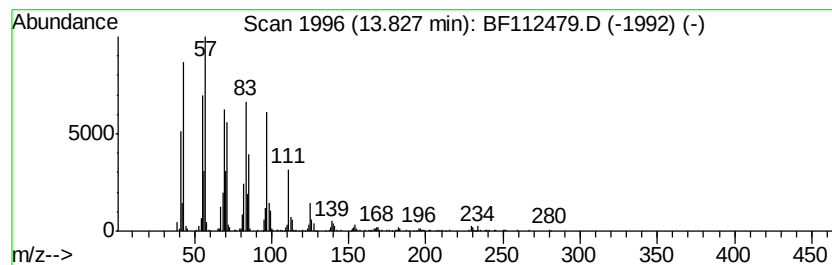
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ClientSampleId :
TEST-PIT-2

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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 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	11.26 ng	790379	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 92
2		Eicosyl pentafluoropropionate	444 C23H41F5O2	1000351-80-8 91
3		Heptafluorobutyric acid, n-octadecyl...	466 C22H37F7O2	000400-57-7 91
4		Eicosyl heptafluorobutyrate	494 C24H41F7O2	1000351-83-5 91
5		Nonadecyl pentafluoropropionate	430 C22H39F5O2	1000351-88-8 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
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Sample : K1452-01
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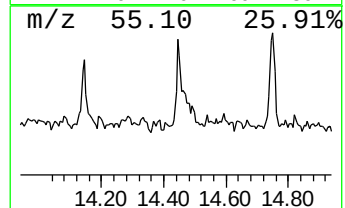
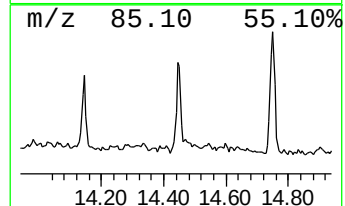
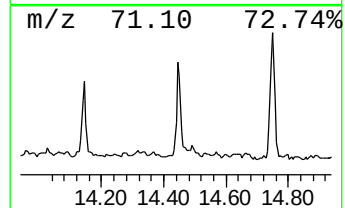
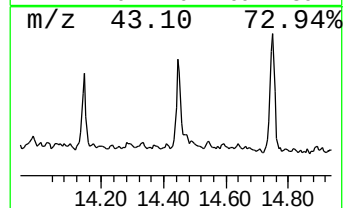
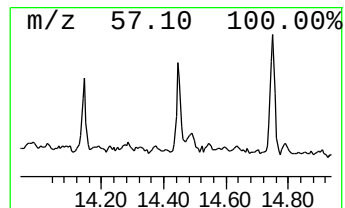
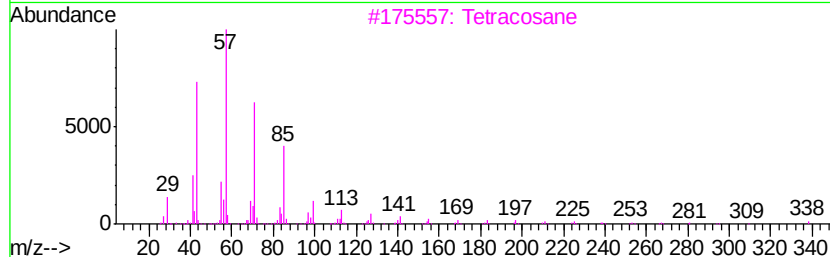
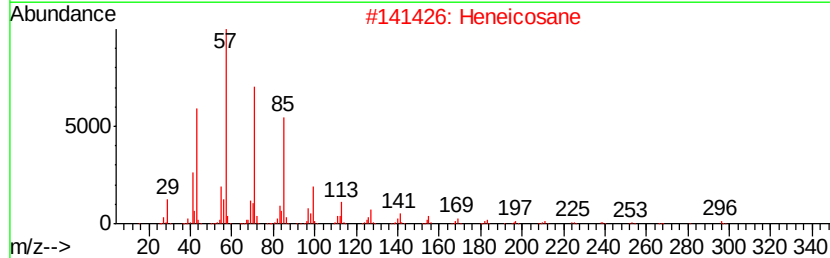
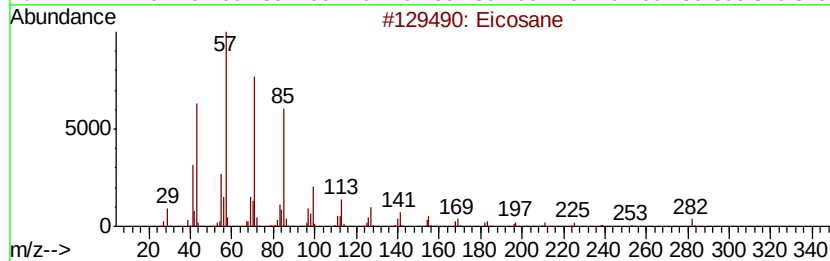
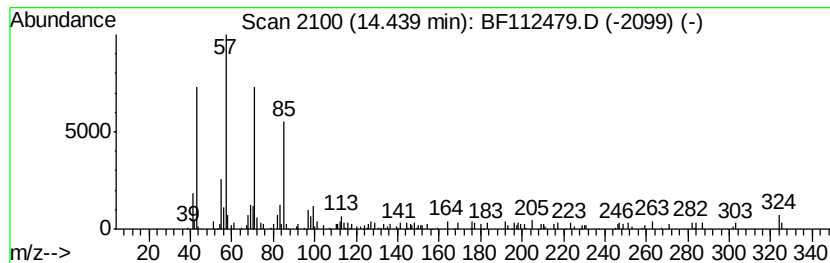
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.55 ng	179236	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 92
2	Heneicosane		296 C21H44	000629-94-7 91
3	Tetracosane		338 C24H50	000646-31-1 90
4	Heptadecane		240 C17H36	000629-78-7 87
5	Hexadecane, 7,9-dimethyl-		254 C18H38	021164-95-4 83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
 Data File : BF112479.D
 Acq On : 11 Feb 2019 14:34
 Operator : JU/SJ
 Sample : K1452-01
 Misc :
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Instrument :
 BNA_F
 ClientSampleId :
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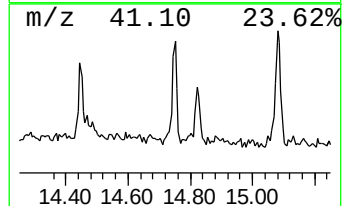
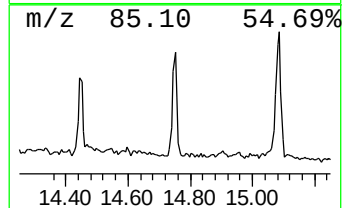
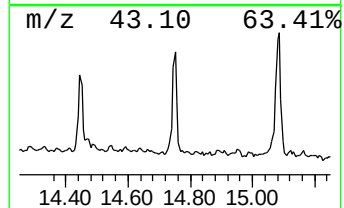
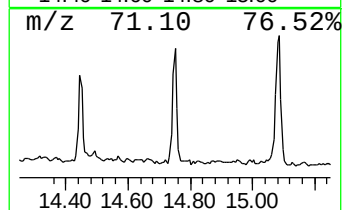
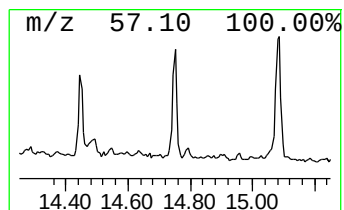
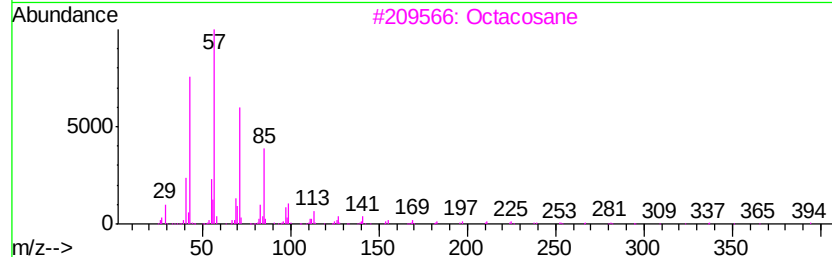
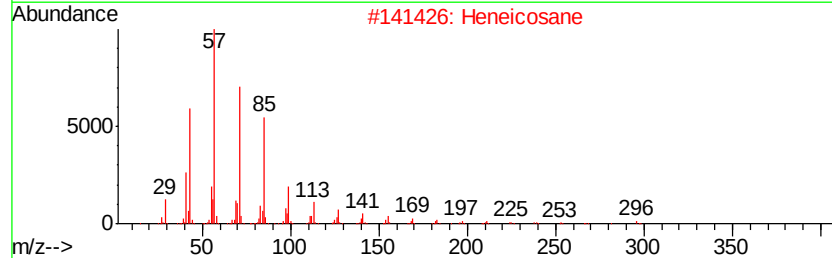
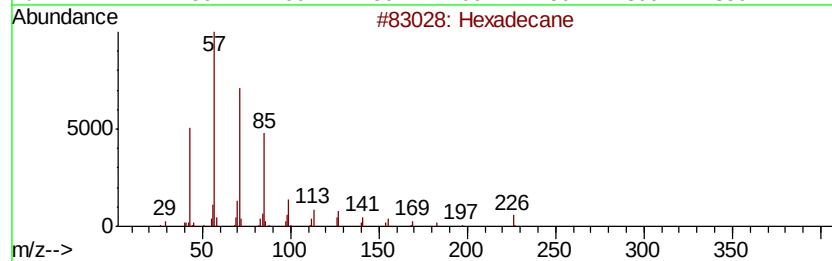
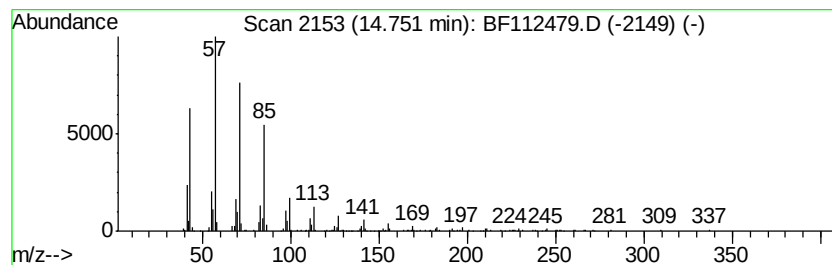
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.79 ng	286867	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112479.D
Acq On : 11 Feb 2019 14:34
Operator : JU/SJ
Sample : K1452-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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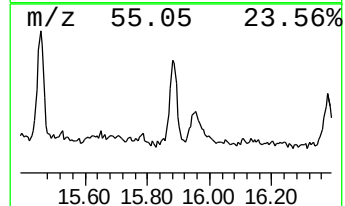
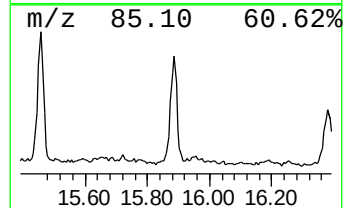
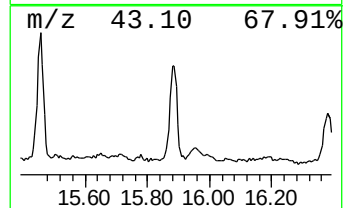
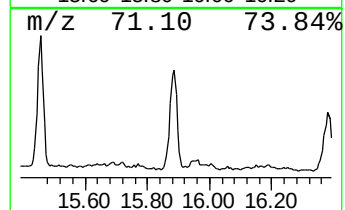
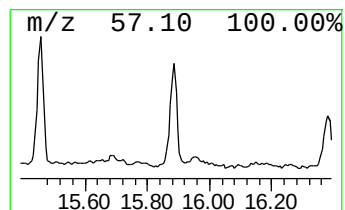
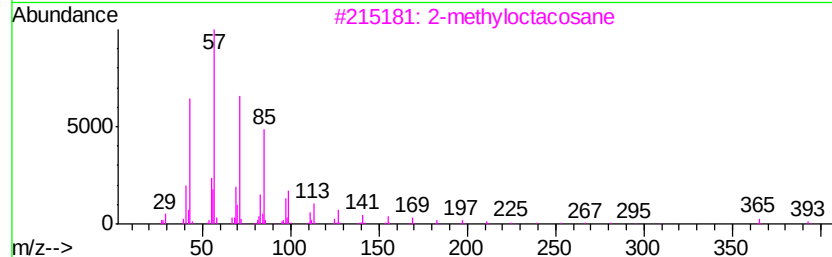
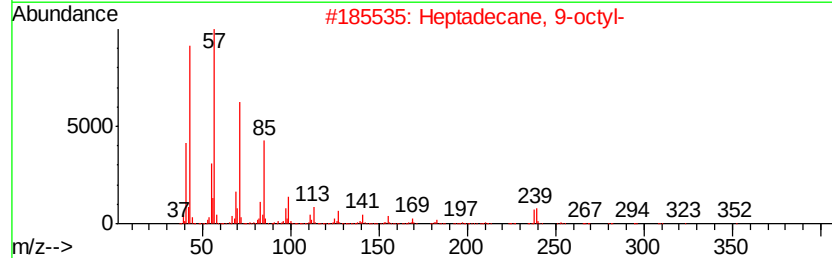
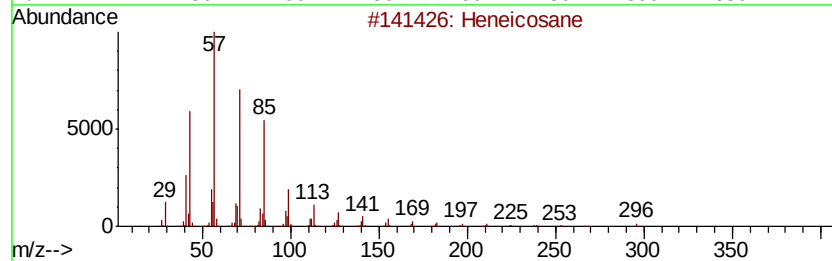
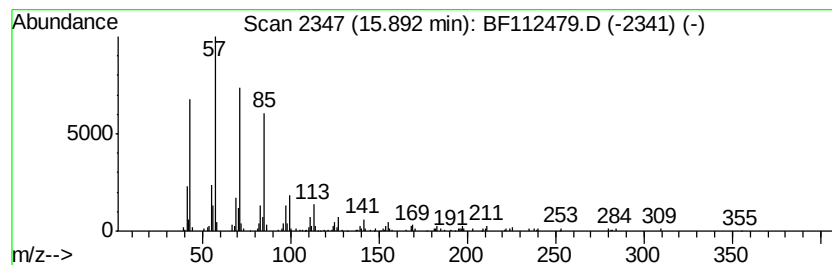
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.79 ng	362587	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Eicosane	282	C20H42	000112-95-8	87
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112479.D
Acq On : 11 Feb 2019 14:34
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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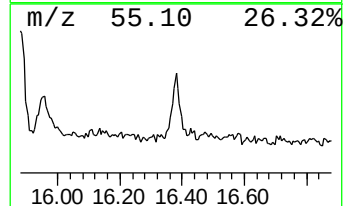
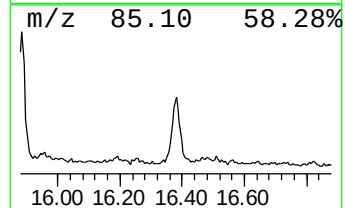
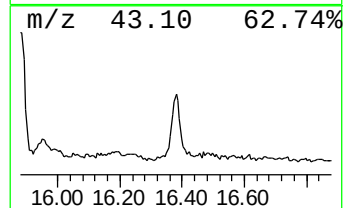
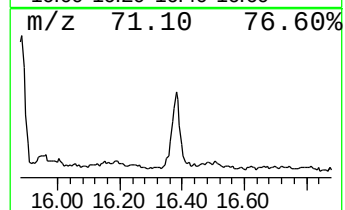
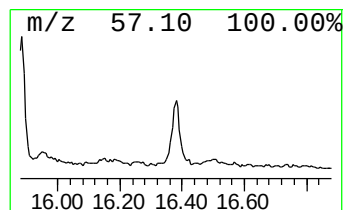
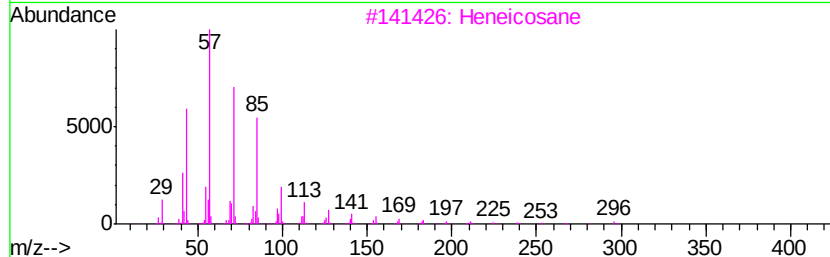
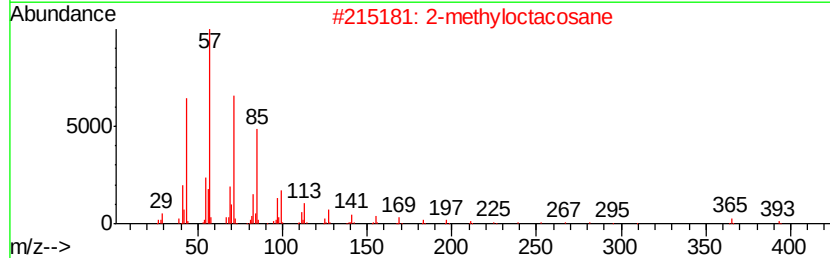
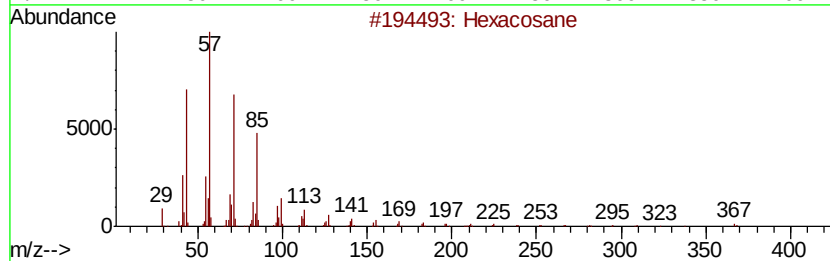
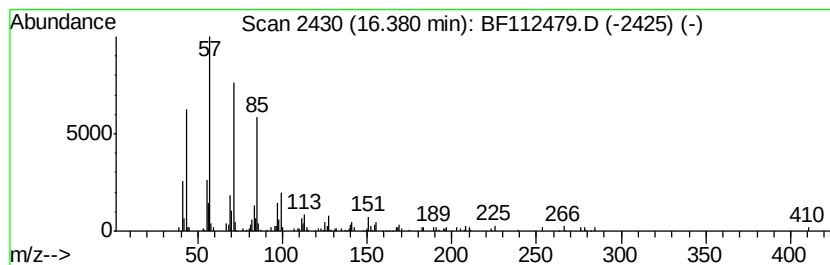
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	3.85 ng	291279	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		2-methyloctacosane	408	C29H60	1000376-72-8	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Hexadecane, 5-butyl-	282	C20H42	006912-07-8	87
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021119\
Data File : BF112479.D
Acq On : 11 Feb 2019 14:34
Operator : JU/SJ
Sample : K1452-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEST-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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2-Pentanone, 4-hy...	5.07	4.4	ng	201050	1	6.83	916599	20.0
unknown6.61	6.61	100.7	ng	4614590	1	6.83	916599	20.0
n-Hexadecanoic acid	11.88	6.8	ng	542944	4	11.36	1602480	20.0
Octadecanoic acid	12.66	5.3	ng	427575	4	11.36	1602480	20.0
1-Heneicosanol	13.83	11.3	ng	790379	5	14.00	1403690	20.0
Eicosane	14.44	2.5	ng	179236	5	14.00	1403690	20.0
Hexadecane	14.75	3.8	ng	286867	6	15.47	1515000	20.0
Heneicosane	15.89	4.8	ng	362587	6	15.47	1515000	20.0
Hexacosane	16.38	3.9	ng	291279	6	15.47	1515000	20.0