

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
 Data File : BF112440.D
 Acq On : 7 Feb 2019 16:12
 Operator : JU/SJ
 Sample : K1401-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200050

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	2.122	3	6	14	rVB	106425	144354	4.67%	0.504%
2	5.057	501	505	515	rVB	86801	121460	3.93%	0.424%
3	5.469	571	575	599	rBV	2584171	2611795	84.44%	9.114%
4	6.481	743	747	759	rBV	2708319	2781637	89.93%	9.707%
5	6.610	765	769	777	rBV	3372688	2900408	93.77%	10.121%
6	6.834	803	807	815	rBV	859458	763756	24.69%	2.665%
7	6.987	829	833	837	rBV	2478176	2200574	71.15%	7.679%
8	7.392	898	902	922	rBV	1656114	1764830	57.06%	6.159%
9	8.116	1021	1025	1041	rBV	970807	1022317	33.05%	3.568%
10	9.186	1202	1207	1219	rBV	3468392	3092974	100.00%	10.793%
11	9.580	1271	1274	1283	rVB	190245	177399	5.74%	0.619%
12	9.869	1319	1323	1327	rBV	1232673	1116390	36.09%	3.896%
13	9.898	1327	1328	1335	rVB	52620	42169	1.36%	0.147%
14	10.416	1413	1416	1421	rVB	42530	43104	1.39%	0.150%
15	10.663	1454	1458	1468	rBV	2227433	2042247	66.03%	7.127%
16	10.780	1474	1478	1485	rVB3	23851	36313	1.17%	0.127%
17	11.357	1572	1576	1579	rBV	1217346	1104056	35.70%	3.853%
18	11.380	1579	1580	1587	rVB	199353	134692	4.35%	0.470%
19	11.704	1630	1635	1638	rVB2	23675	34607	1.12%	0.121%
20	11.880	1659	1665	1672	rBV3	228735	323715	10.47%	1.130%
21	11.974	1678	1681	1690	rVB2	39783	54556	1.76%	0.190%
22	12.574	1779	1783	1788	rBV	153355	161024	5.21%	0.562%
23	12.663	1795	1798	1804	rBV2	37554	53993	1.75%	0.188%
24	12.804	1816	1822	1825	rBV	122517	155824	5.04%	0.544%
25	12.939	1840	1845	1848	rBV	2565653	2448778	79.17%	8.545%
26	13.821	1990	1995	2007	rBV3	257346	391001	12.64%	1.364%
27	13.998	2021	2025	2029	rBV	970518	958535	30.99%	3.345%
28	14.027	2029	2030	2037	rVB	64171	41288	1.33%	0.144%
29	14.145	2046	2050	2056	rBV2	71239	88675	2.87%	0.309%
30	14.451	2098	2102	2107	rBV	90513	110771	3.58%	0.387%
31	14.751	2150	2153	2159	rVB	96223	106667	3.45%	0.372%
32	14.827	2162	2166	2172	rVB	419632	411193	13.29%	1.435%
33	15.045	2200	2203	2206	rBV	37628	54523	1.76%	0.190%
34	15.086	2206	2210	2213	rVB2	97541	119965	3.88%	0.419%

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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	15.468	2270	2275	2285	rBV	628335	901055	29.13%	3.144%
36	15.886	2342	2346	2351	rVB	65260	86279	2.79%	0.301%
37	16.962	2525	2529	2535	rVB8	30877	53232	1.72%	0.186%

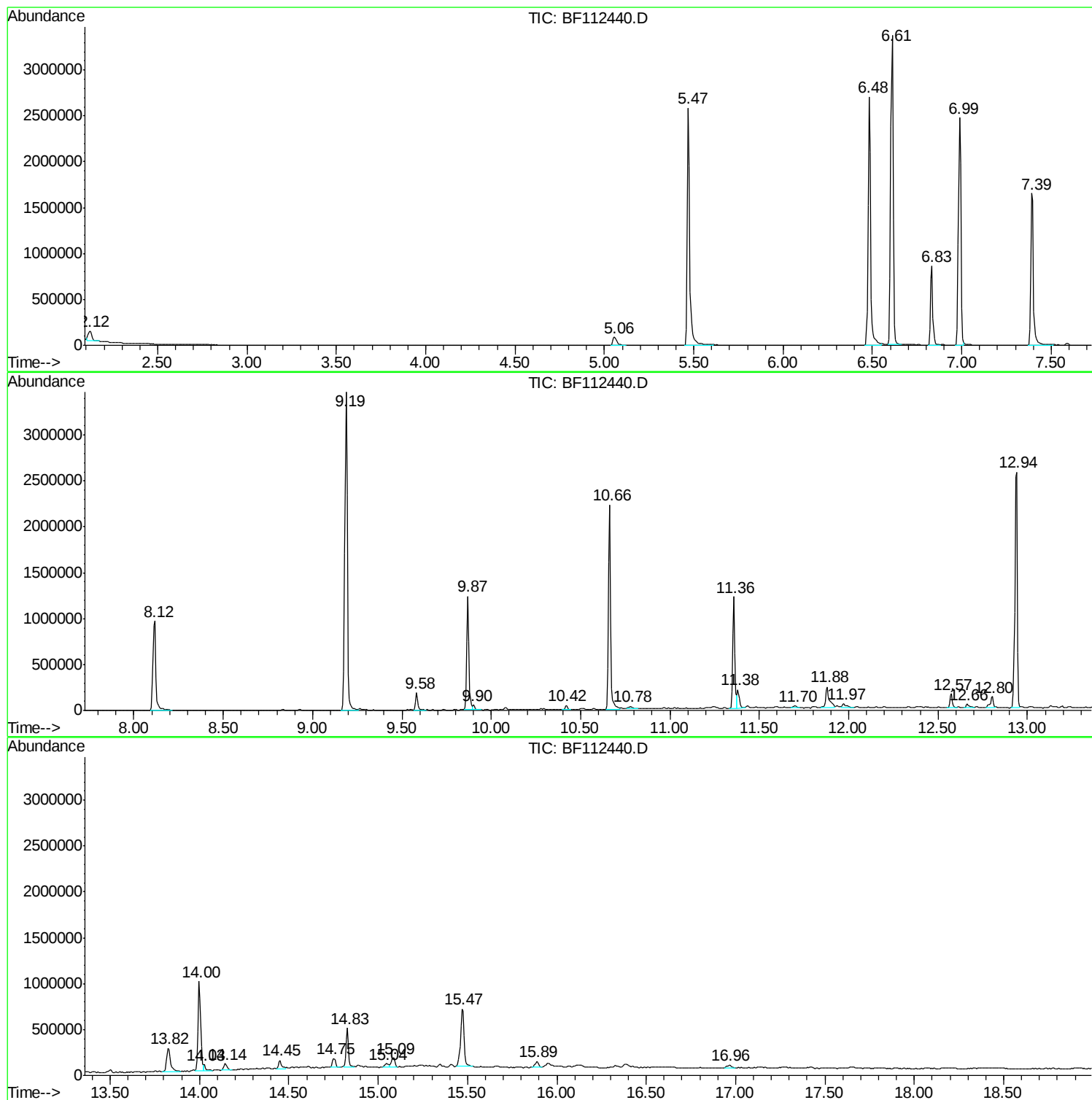
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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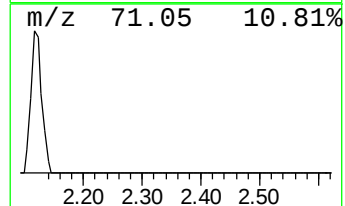
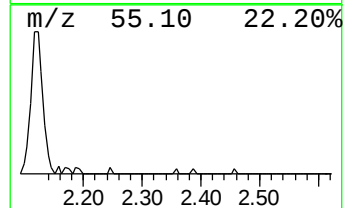
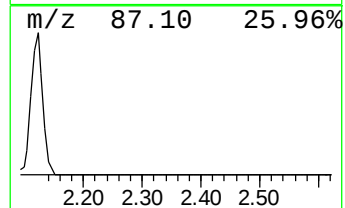
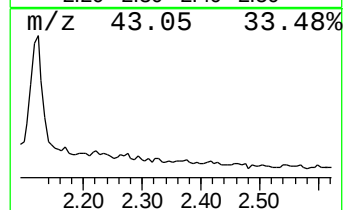
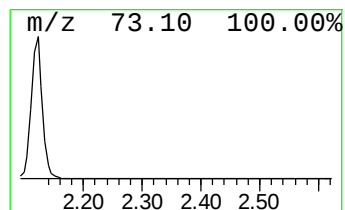
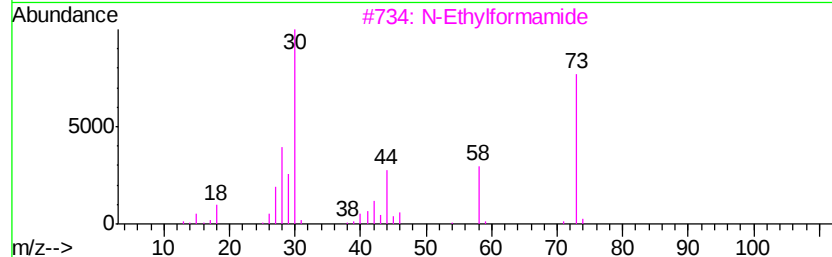
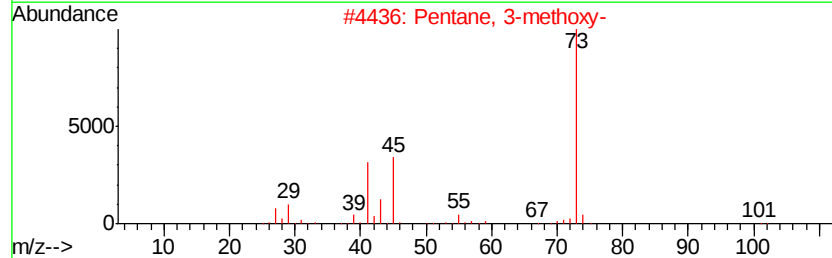
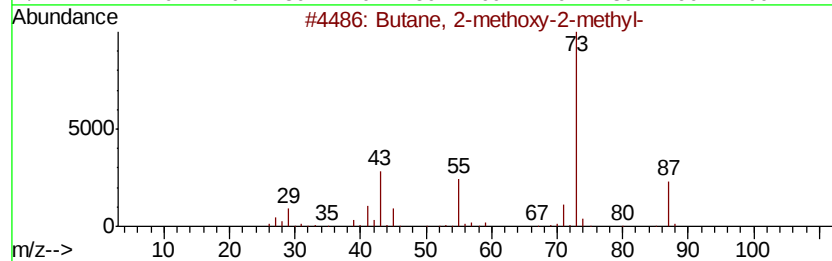
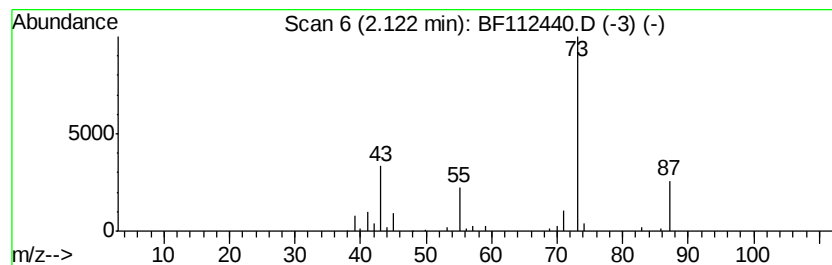
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	3.78 ng	144354	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	72
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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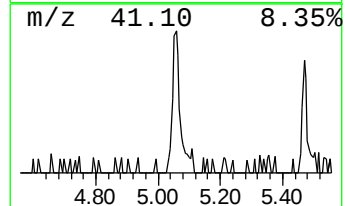
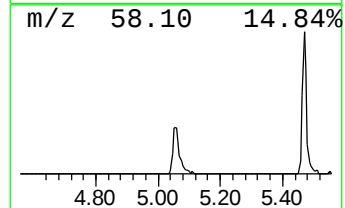
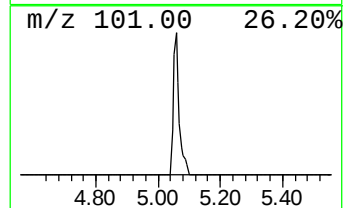
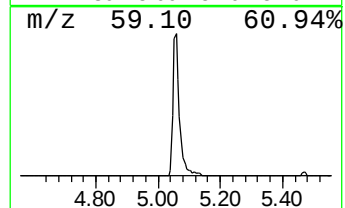
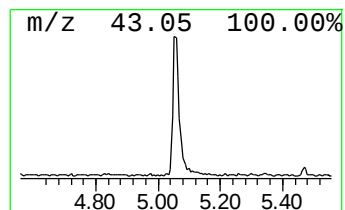
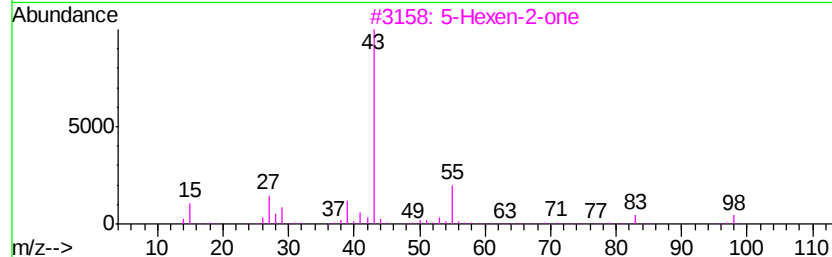
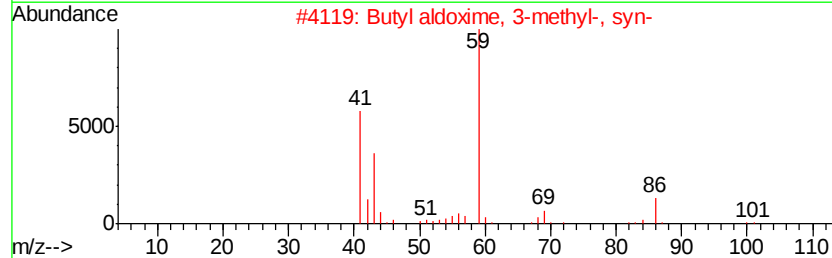
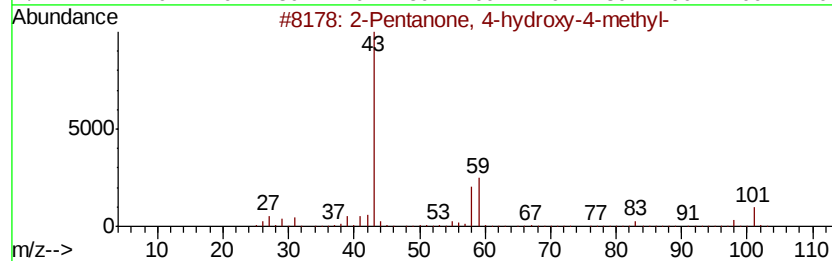
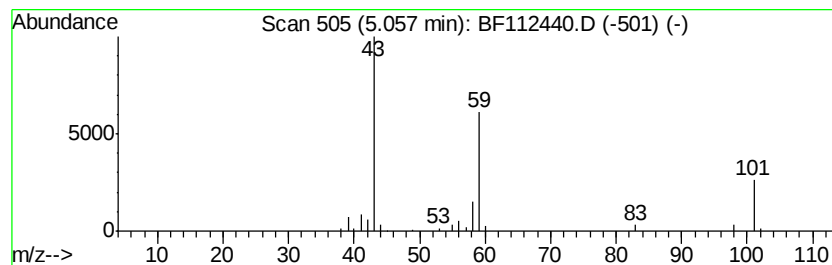
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.18 ng	121460	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		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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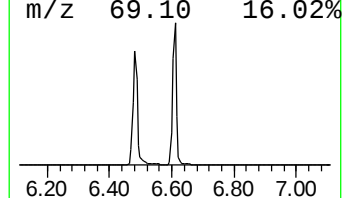
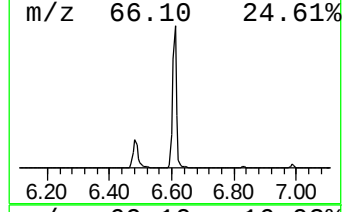
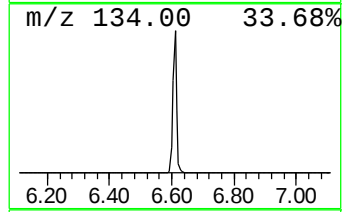
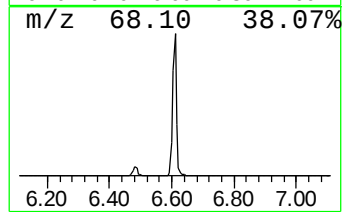
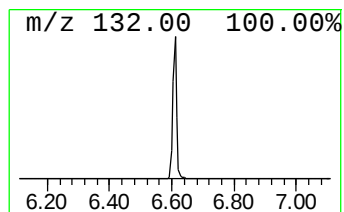
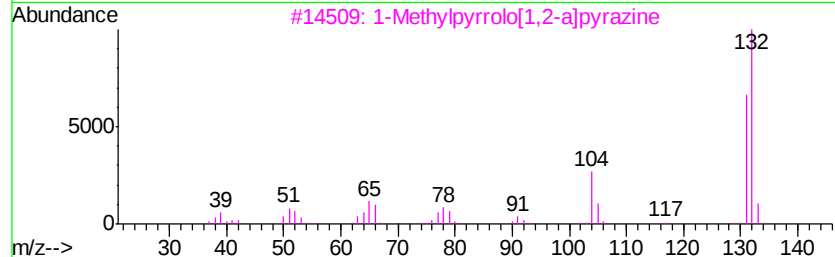
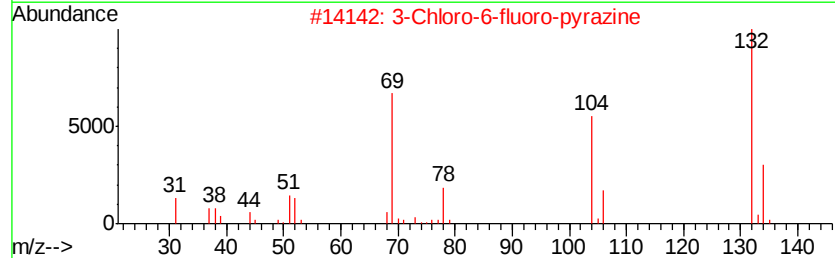
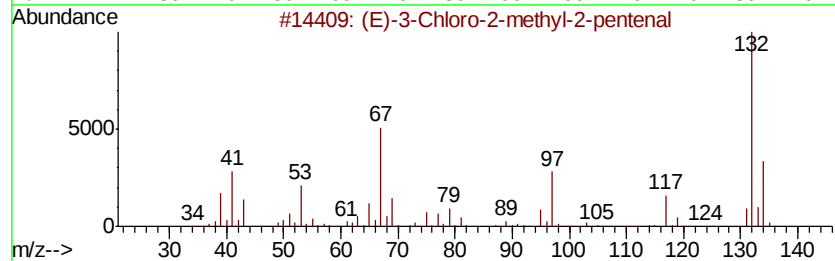
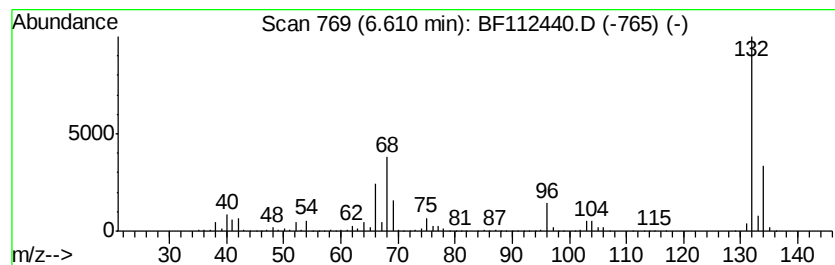
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	75.95 ng	2900410	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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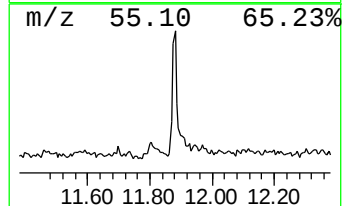
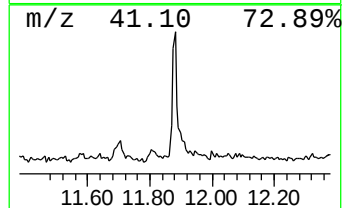
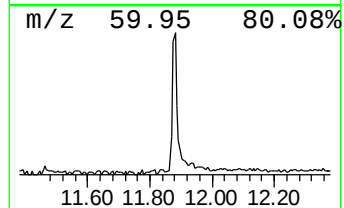
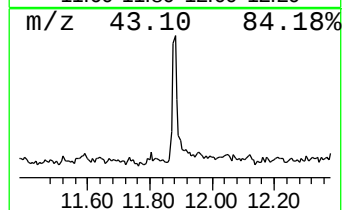
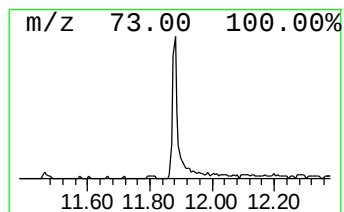
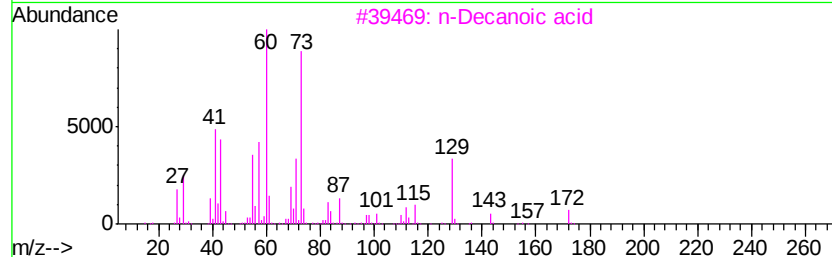
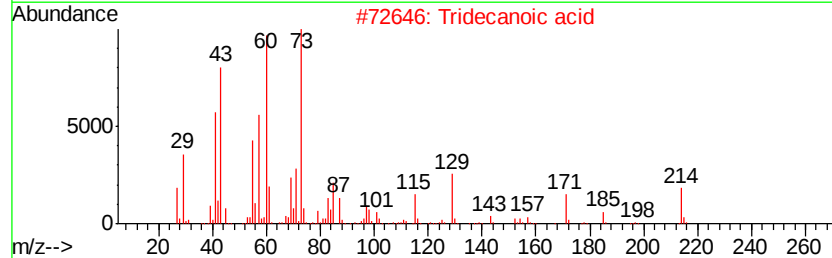
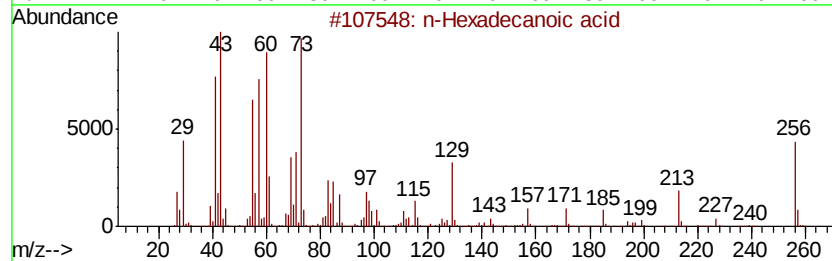
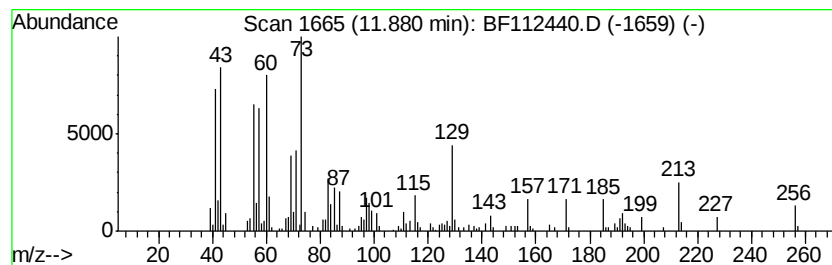
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.88	5.86 ng	323715	Phenanthrene-d10		11.36	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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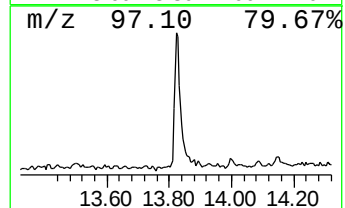
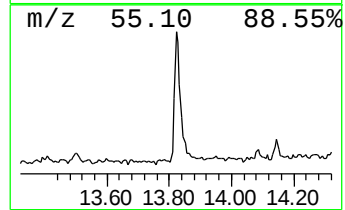
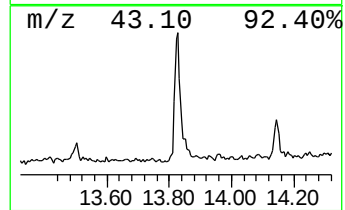
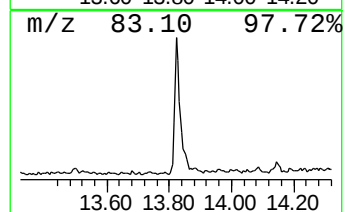
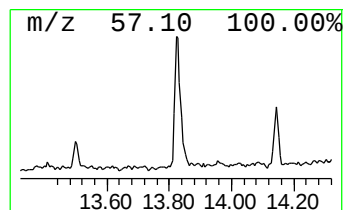
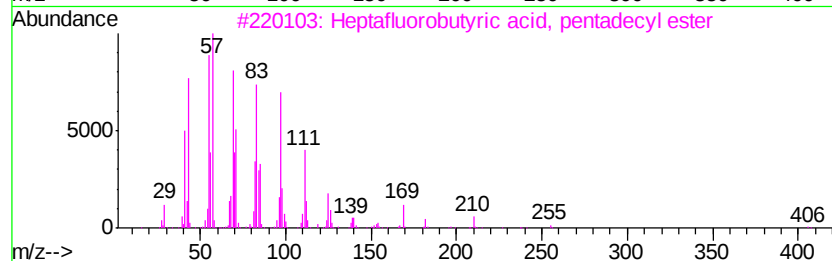
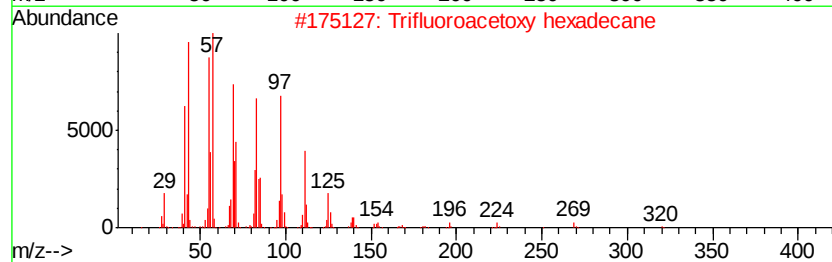
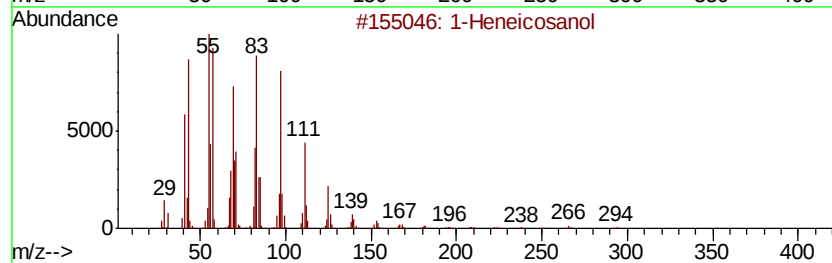
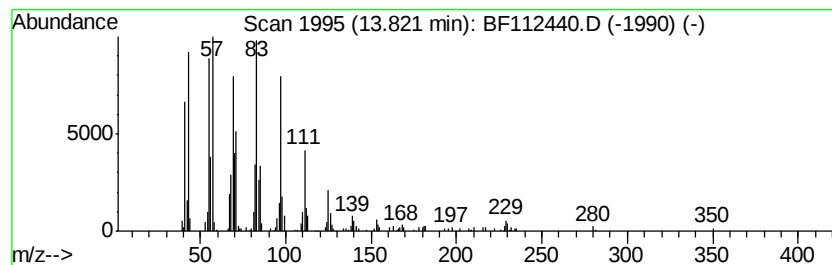
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	8.16 ng	391001	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	1	Heptafluorobutyric acid, pentadecyl...	424	C19H31F7O2	959261-23-5	93
4	1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112440.D
Acq On : 7 Feb 2019 16:12
Operator : JU/SJ
Sample : K1401-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200050

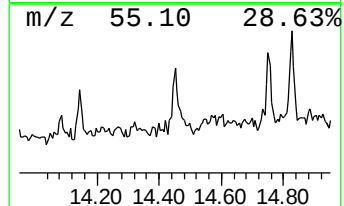
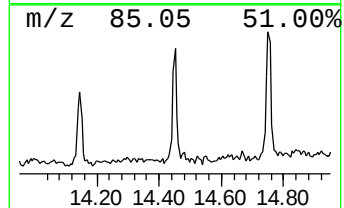
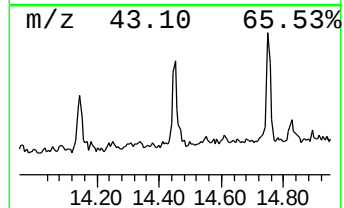
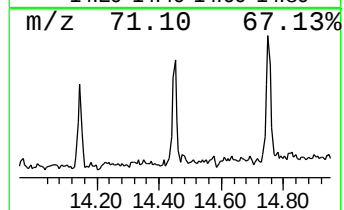
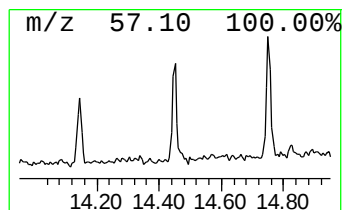
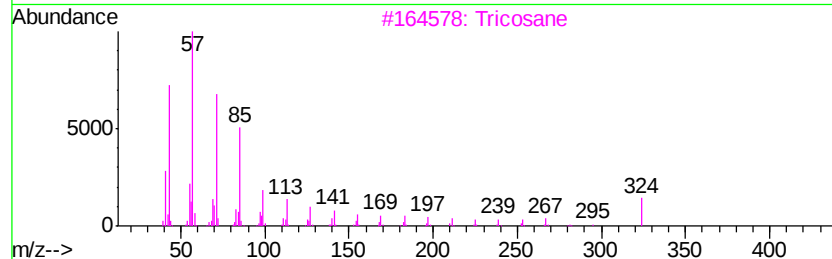
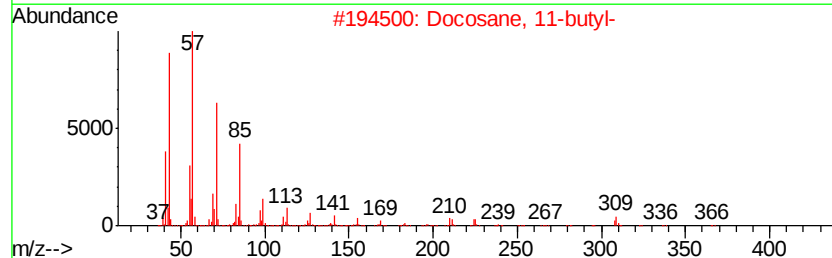
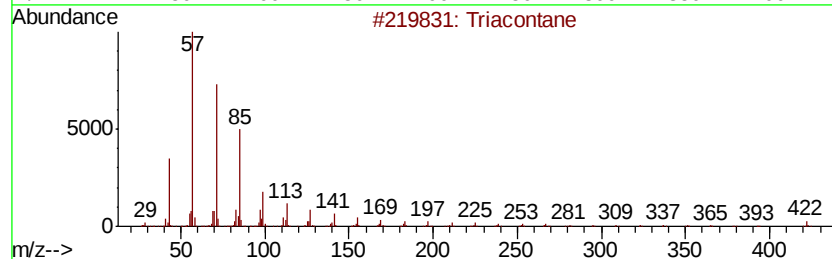
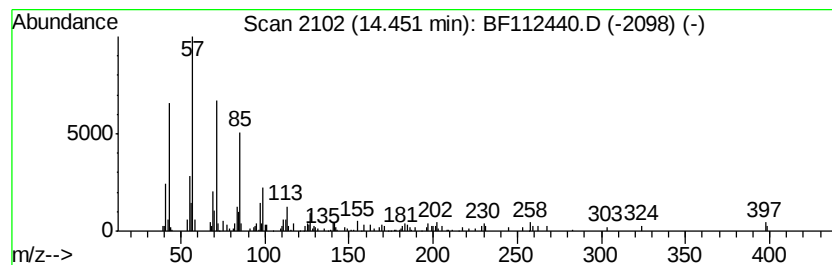
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.31 ng	110771	Chrysene-d12	14.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	87
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	86
3			Tricosane	324	C23H48	000638-67-5	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112440.D
Acq On : 7 Feb 2019 16:12
Operator : JU/SJ
Sample : K1401-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200050

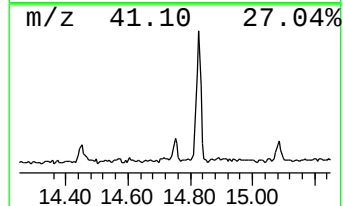
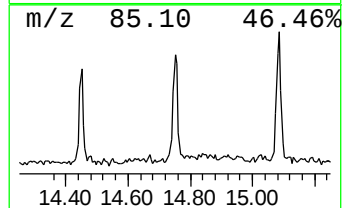
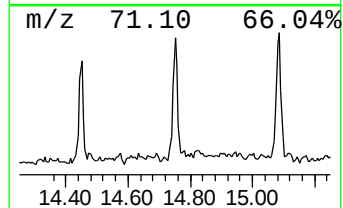
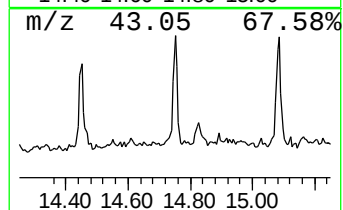
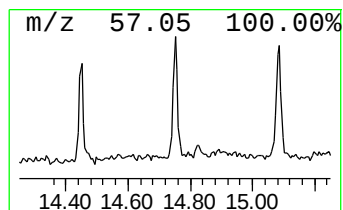
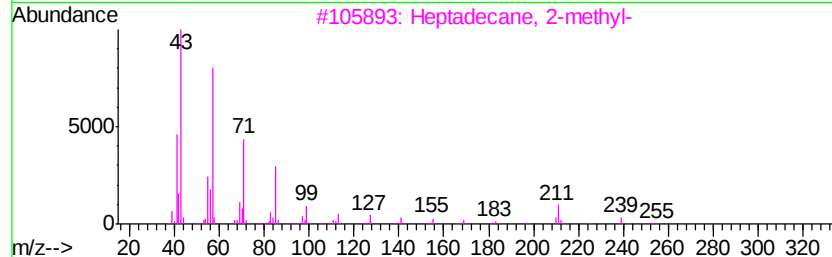
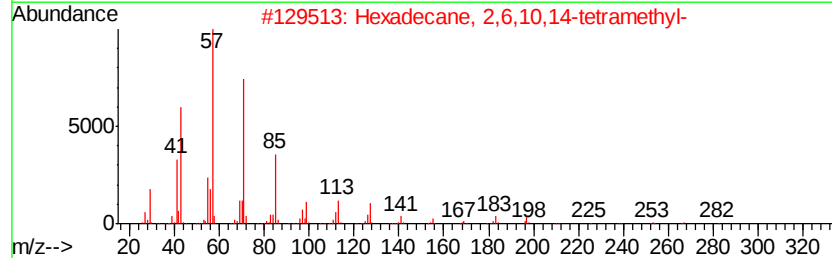
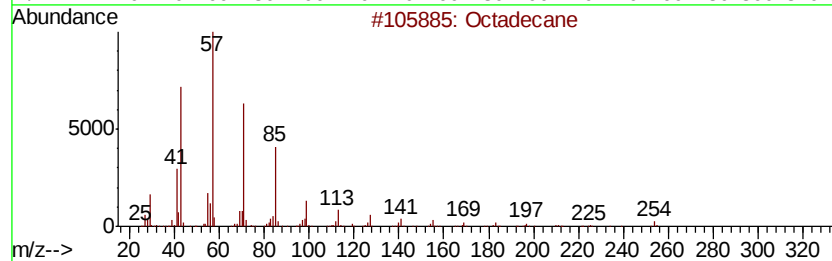
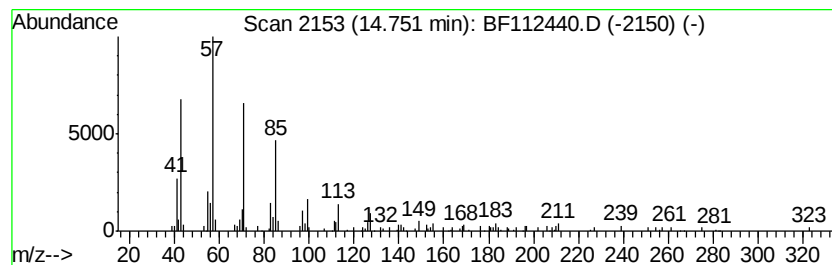
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.37 ng	106667	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	96
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93
3		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112440.D
Acq On : 7 Feb 2019 16:12
Operator : JU/SJ
Sample : K1401-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200050

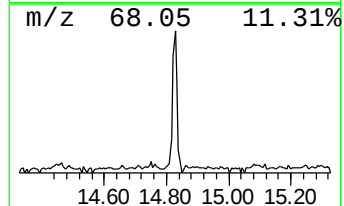
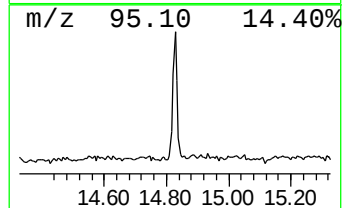
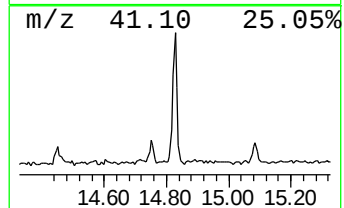
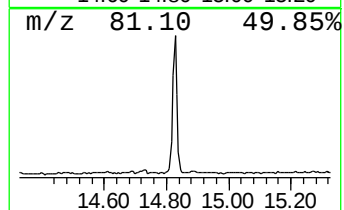
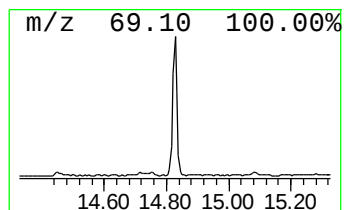
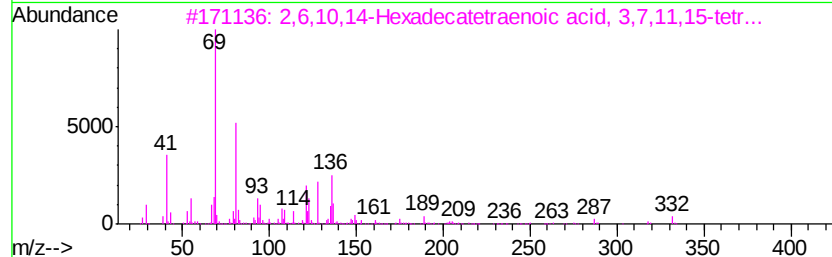
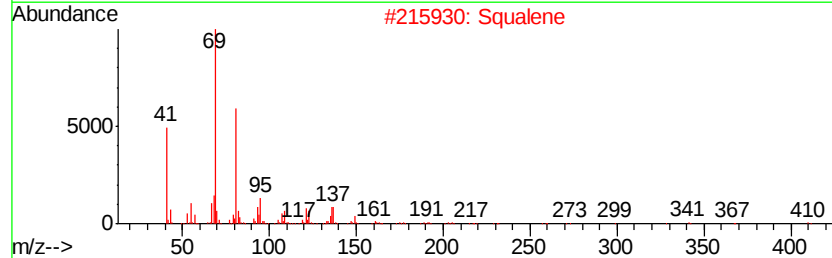
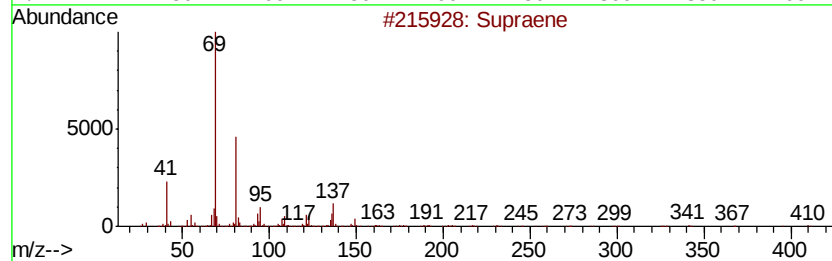
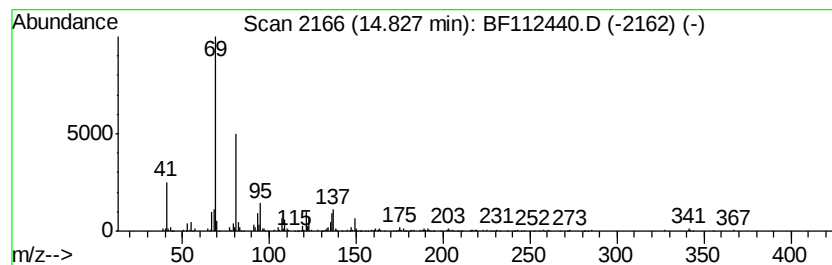
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	9.13 ng	411193	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		Acetic acid, 1,3,7-trimethylocta...	210	C13H22O2	091418-25-6	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112440.D
Acq On : 7 Feb 2019 16:12
Operator : JU/SJ
Sample : K1401-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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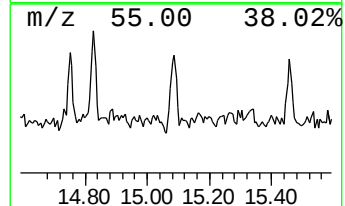
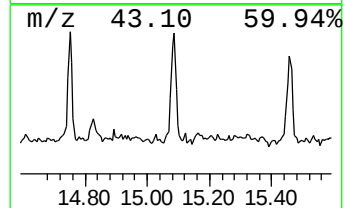
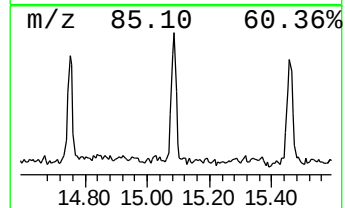
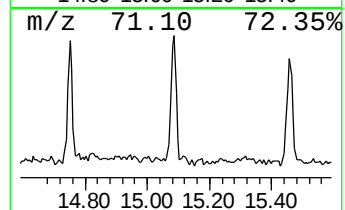
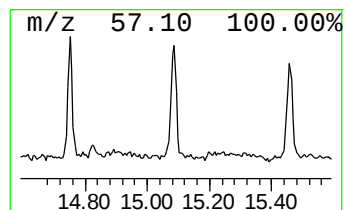
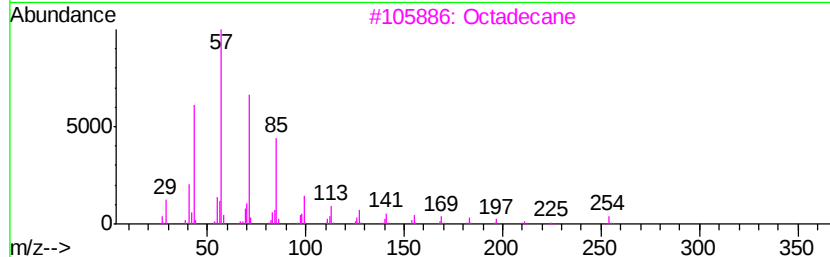
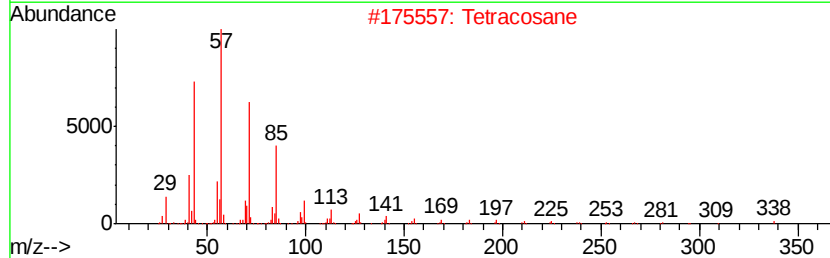
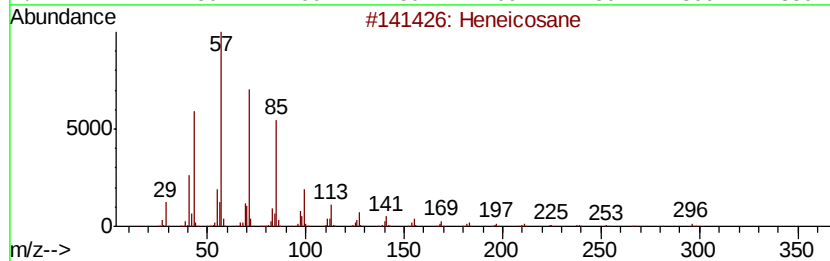
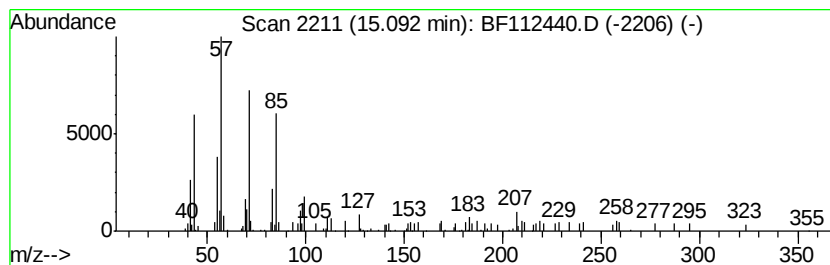
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.66 ng	119965	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Tetracosane	338	C24H50	000646-31-1	90
3		Octadecane	254	C18H38	000593-45-3	86
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5		Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
Data File : BF112440.D
Acq On : 7 Feb 2019 16:12
Operator : JU/SJ
Sample : K1401-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.06	3.2	ng	121460	1	6.83	763756	20.0
unknown6.61	6.61	76.0	ng	2900410	1	6.83	763756	20.0
n-Hexadecanoic acid	11.88	5.9	ng	323715	4	11.36	1104060	20.0
1-Heneicosanol	13.82	8.2	ng	391001	5	14.00	958535	20.0
Triacontane	14.45	2.3	ng	110771	5	14.00	958535	20.0
Octadecane	14.75	2.4	ng	106667	6	15.47	901055	20.0
Supraene	14.83	9.1	ng	411193	6	15.47	901055	20.0
Heneicosane	15.09	2.7	ng	119965	6	15.47	901055	20.0