

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012519\
 Data File : BF112241.D
 Acq On : 25 Jan 2019 19:32
 Operator : JU/SJ
 Sample : K1238-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S2

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

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	2.163	6	13	19	rVB	158049	202231	3.81%	0.412%
2	5.081	504	509	521	rVB	140449	220490	4.15%	0.449%
3	5.487	573	578	581	rBV	3841947	3735462	70.34%	7.613%
4	6.492	743	749	752	rBV	4338992	5054644	95.18%	10.302%
5	6.622	766	771	774	rBV	5517085	5310348	100.00%	10.823%
6	6.675	777	780	791	rVB	43098	68220	1.28%	0.139%
7	6.840	805	808	816	rBV	1186329	1089060	20.51%	2.220%
8	6.998	831	835	839	rBV	4234103	4143361	78.02%	8.445%
9	7.404	899	904	907	rBV	3053902	3300886	62.16%	6.728%
10	8.122	1022	1026	1042	rBV	1344160	1270887	23.93%	2.590%
11	9.198	1203	1209	1212	rBV	5412843	4984911	93.87%	10.160%
12	9.586	1271	1275	1280	rBV	472061	397114	7.48%	0.809%
13	9.881	1320	1325	1328	rBV	1681256	1586798	29.88%	3.234%
14	10.669	1455	1459	1473	rBV	3719939	3826265	72.05%	7.798%
15	11.363	1573	1577	1584	rBV	1810029	1597717	30.09%	3.256%
16	11.886	1663	1666	1675	rBV2	131764	155141	2.92%	0.316%
17	12.574	1780	1783	1787	rBV	58769	58113	1.09%	0.118%
18	12.827	1817	1826	1835	rBV2	445181	889625	16.75%	1.813%
19	12.945	1841	1846	1849	rBV	5071365	4840306	91.15%	9.865%
20	13.169	1879	1884	1887	rVB	67516	67911	1.28%	0.138%
21	13.510	1936	1942	1944	rBV2	101042	100054	1.88%	0.204%
22	13.839	1991	1998	2007	rBV2	294274	409026	7.70%	0.834%
23	13.998	2022	2025	2029	rBV	990957	998044	18.79%	2.034%
24	14.151	2047	2051	2055	rBV	192117	187670	3.53%	0.382%
25	14.457	2099	2103	2106	rBV	298236	268539	5.06%	0.547%
26	14.763	2149	2155	2159	rBV	429738	487915	9.19%	0.994%
27	15.092	2206	2211	2219	rVB	597950	696632	13.12%	1.420%
28	15.468	2269	2275	2284	rBV2	1321927	1842696	34.70%	3.756%
29	15.898	2342	2348	2357	rBV	448809	696087	13.11%	1.419%
30	16.398	2427	2433	2440	rBV	209313	374297	7.05%	0.763%
31	16.986	2528	2533	2542	rVB3	82140	204794	3.86%	0.417%

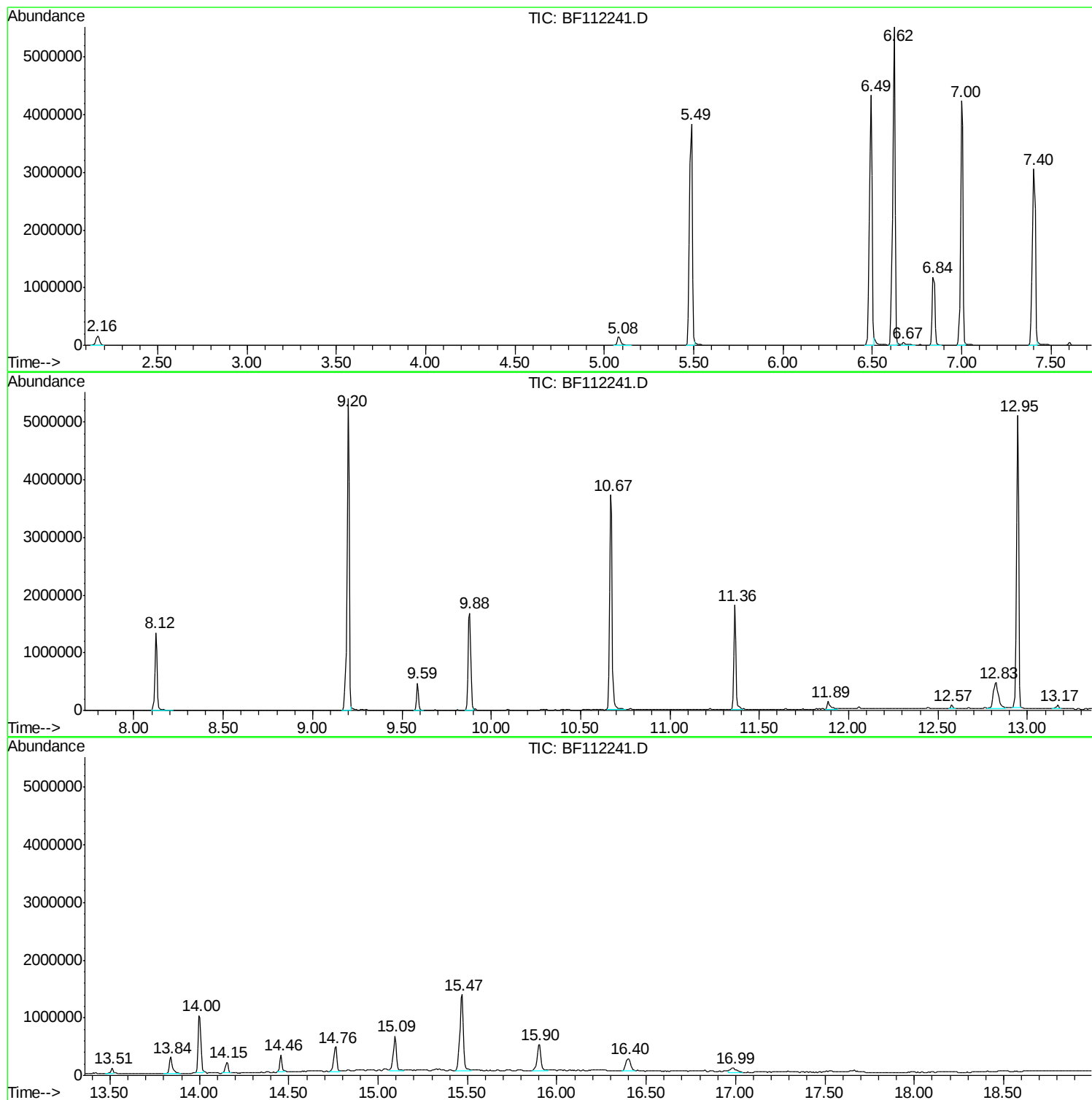
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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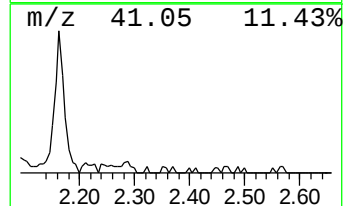
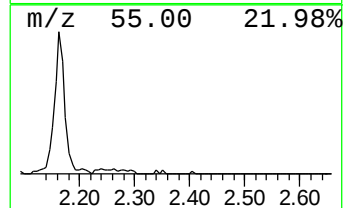
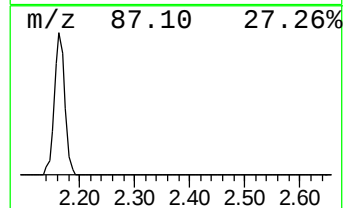
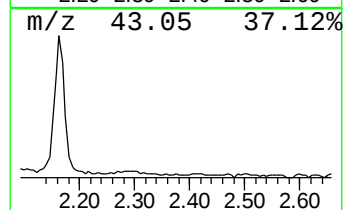
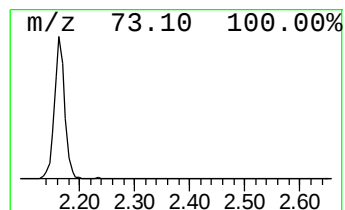
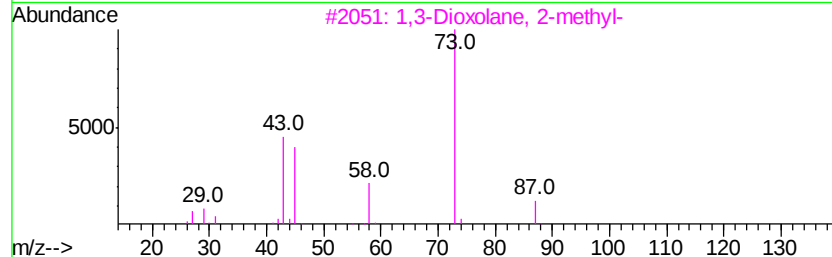
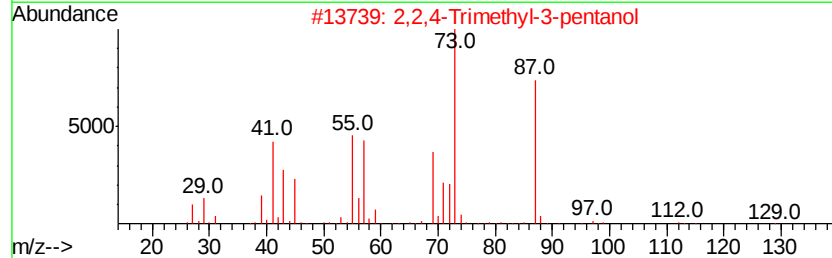
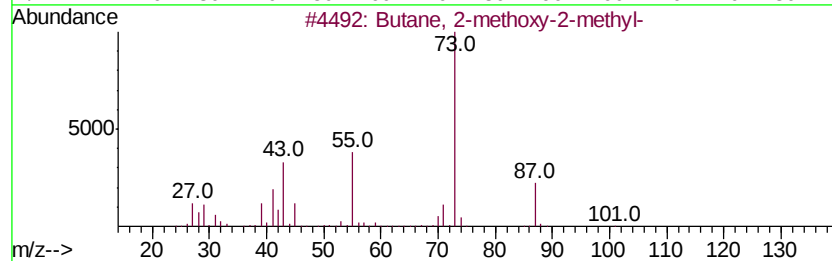
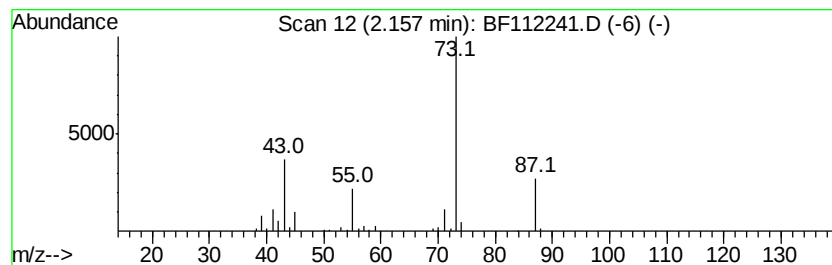
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.71 ng	202231	1,4-Dichlorobenzene-d4	6.84

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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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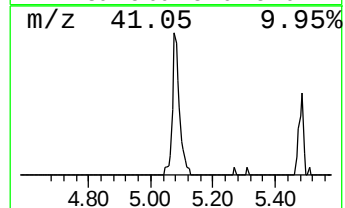
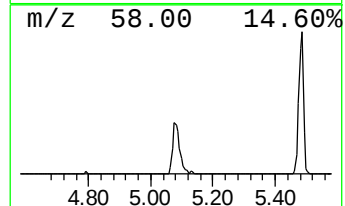
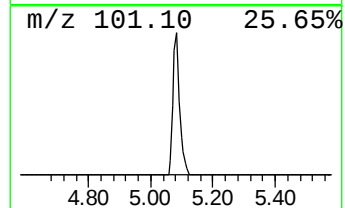
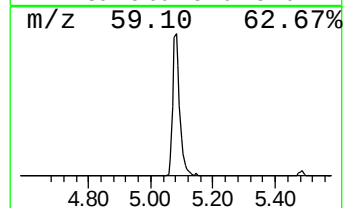
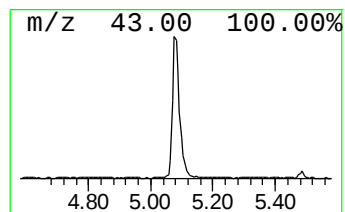
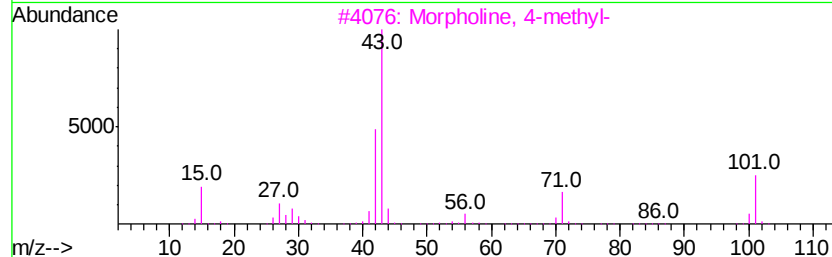
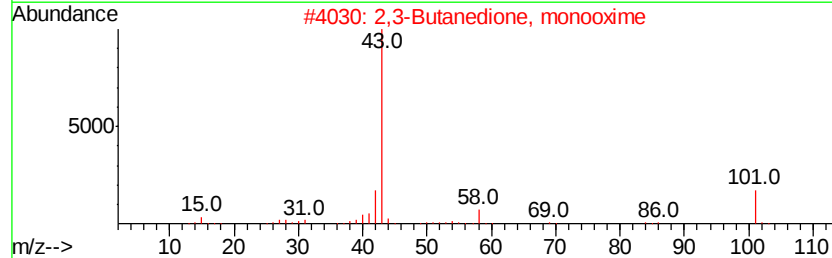
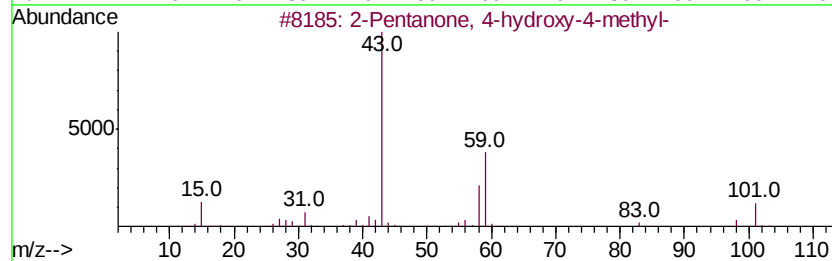
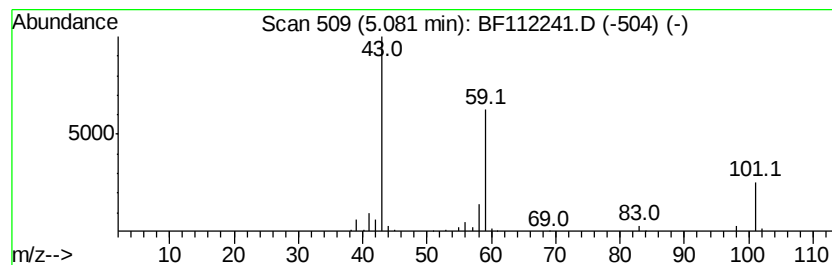
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.05 ng	220490	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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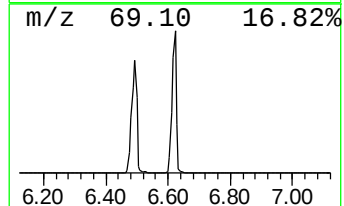
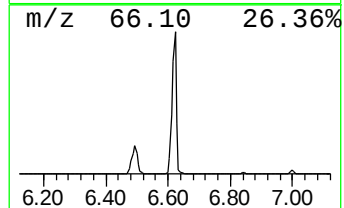
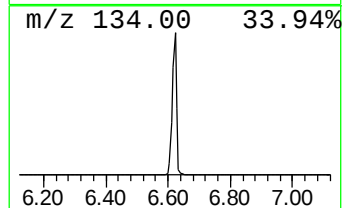
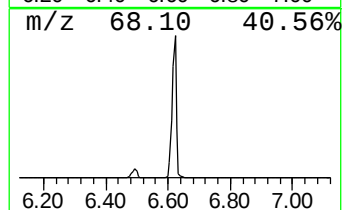
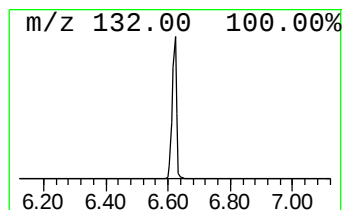
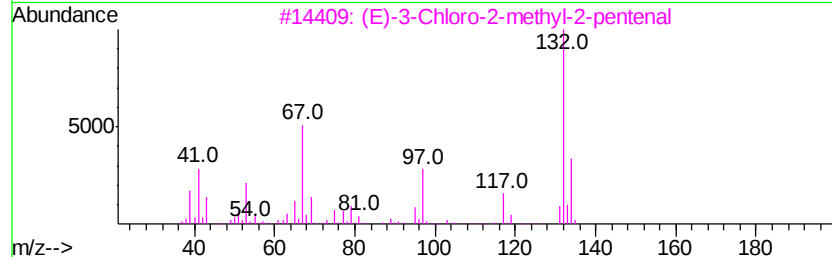
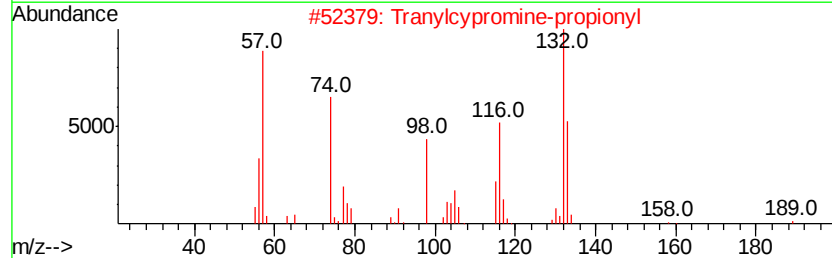
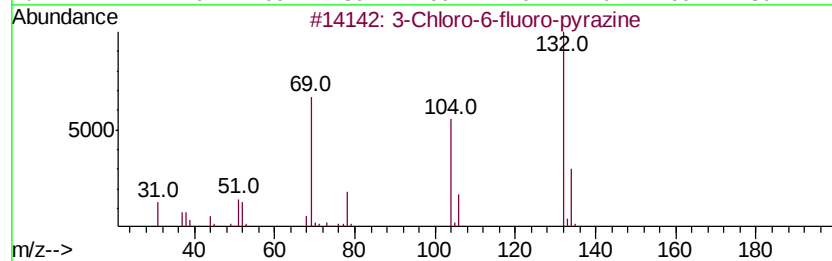
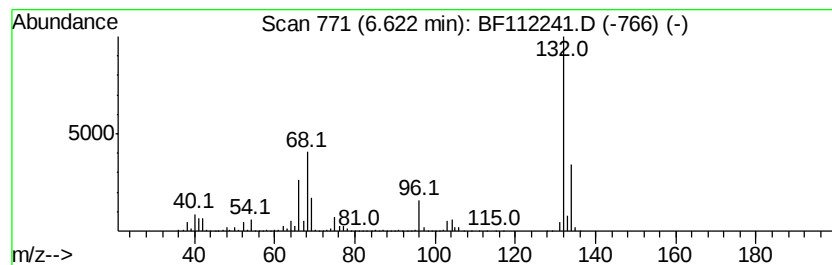
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	97.52 ng	5310350	1,4-Dichlorobenzene-d4	6.84

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	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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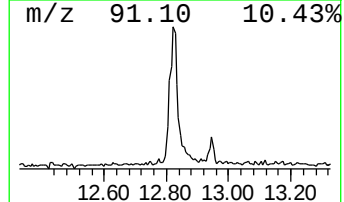
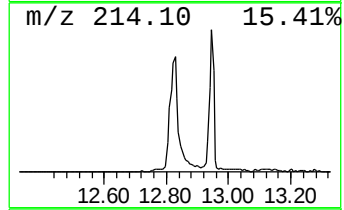
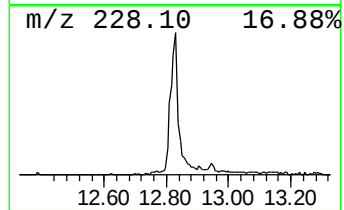
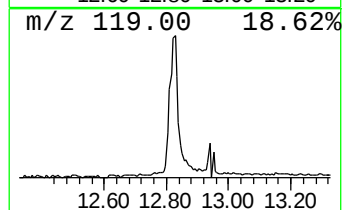
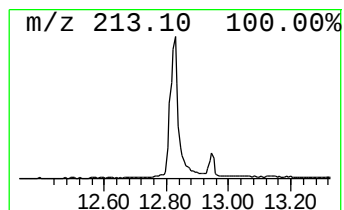
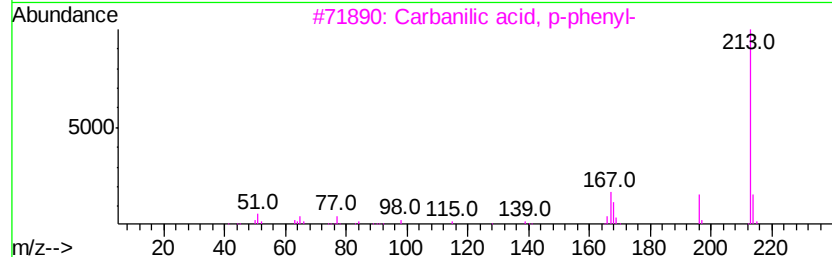
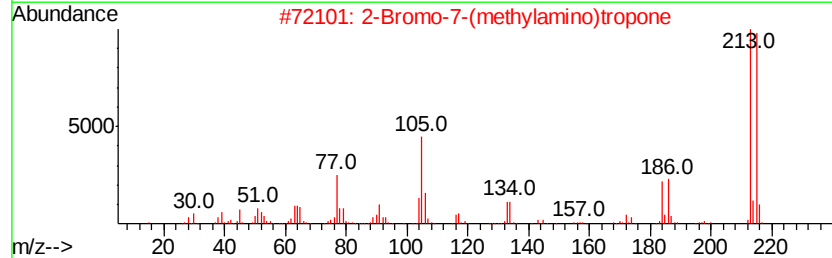
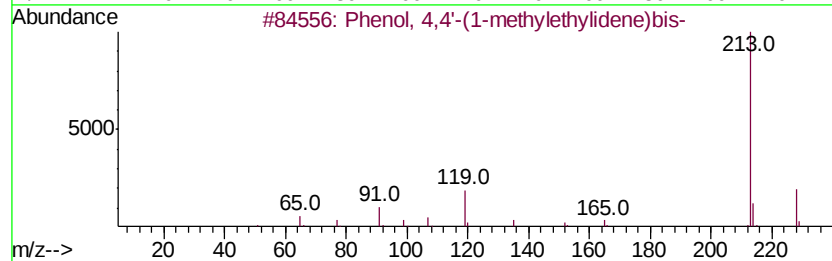
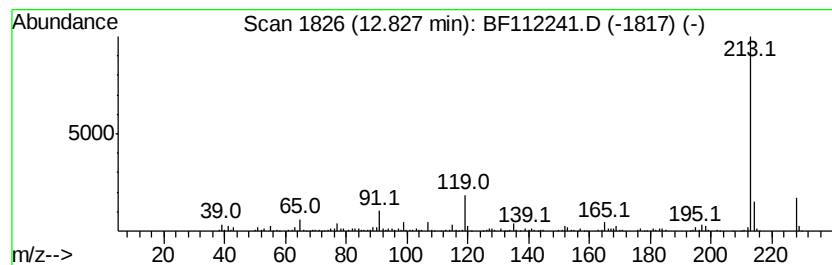
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Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	17.83 ng	889625	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	97
2		2-Bromo-7-(methylamino)tropone	213	C8H8BrNO	103539-25-9	53
3		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
4		1,4-Naphthalenedione, 2-(1-butenyl)-	228	C14H12O3	029366-43-6	50
5		2-Trifluoromethyl-5-hydroxyquino-	213	C10H6F3NO	041958-06-9	50



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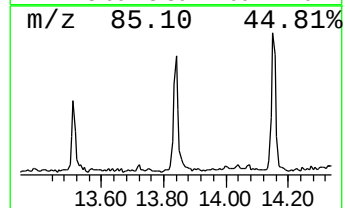
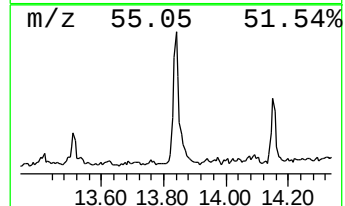
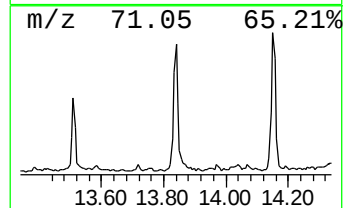
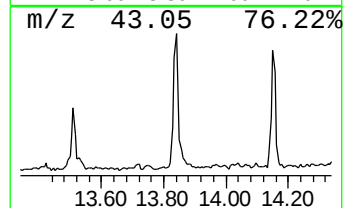
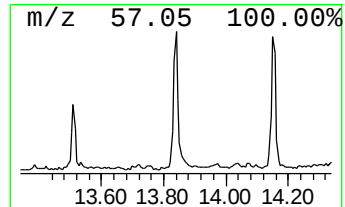
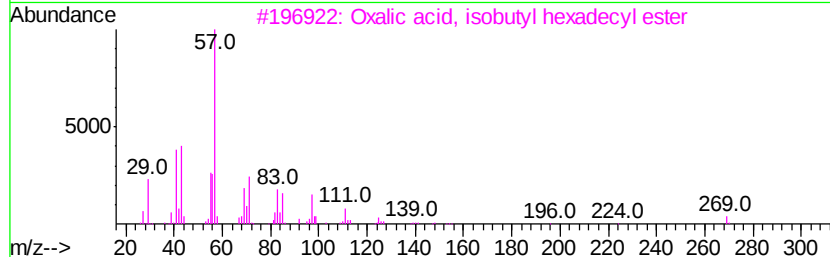
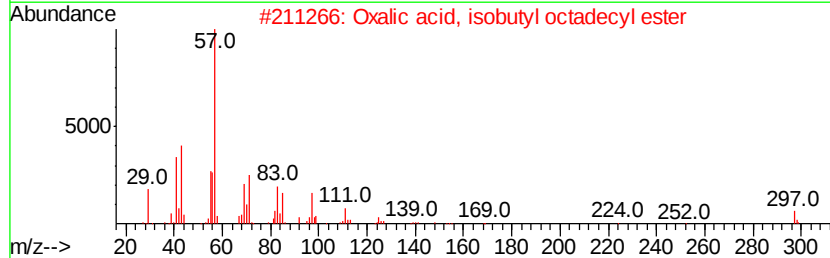
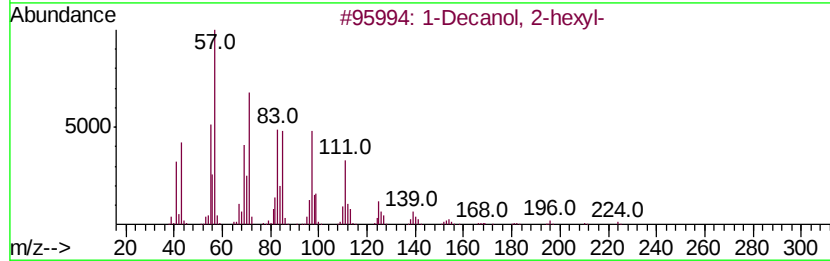
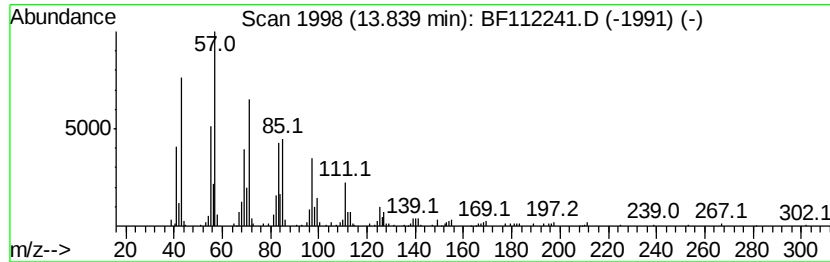
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	8.20 ng	409026	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
5		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91



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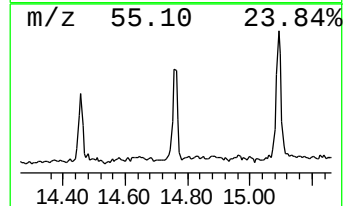
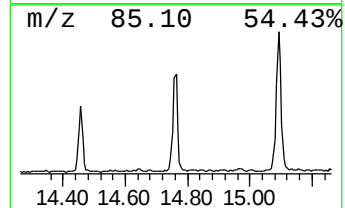
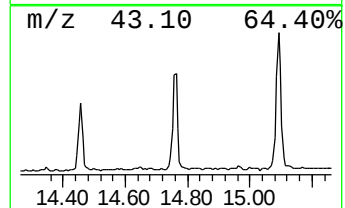
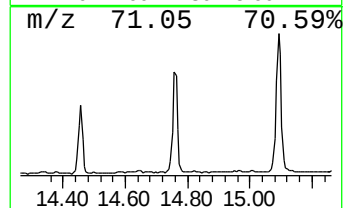
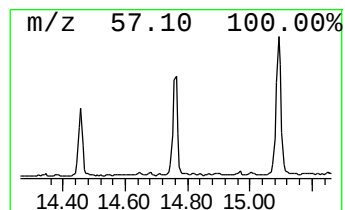
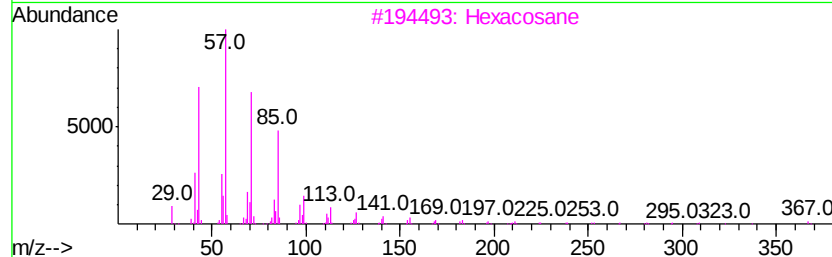
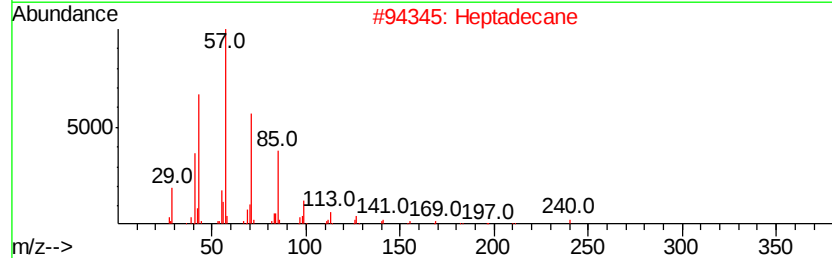
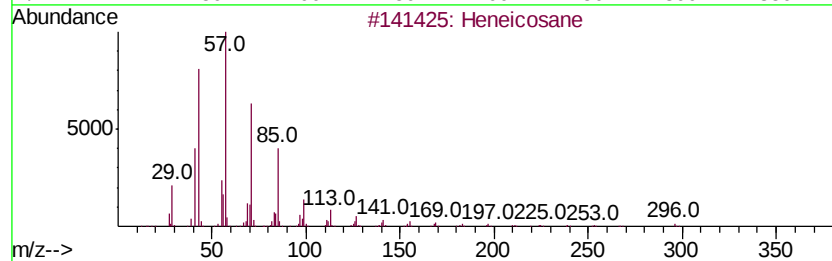
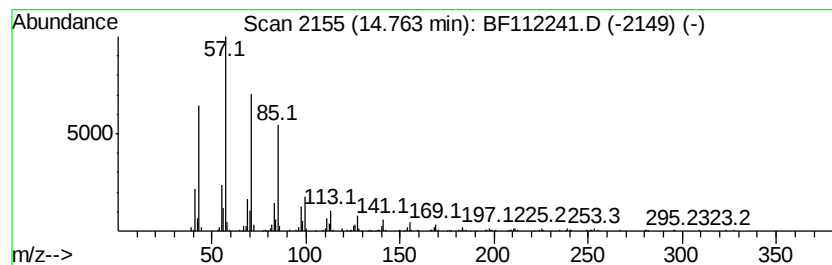
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	5.30 ng	487915	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Heptadecane		240	C17H36	000629-78-7	94
3	Hexacosane		366	C26H54	000630-01-3	93
4	Eicosane		282	C20H42	000112-95-8	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012519\
Data File : BF112241.D
Acq On : 25 Jan 2019 19:32
Operator : JU/SJ
Sample : K1238-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

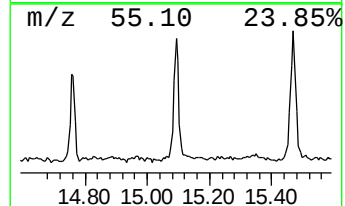
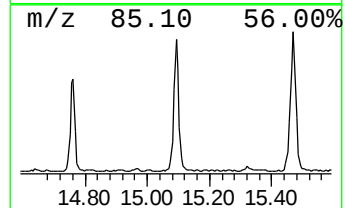
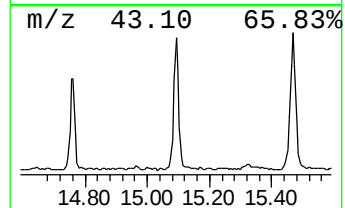
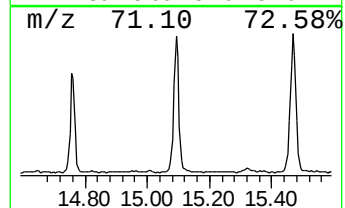
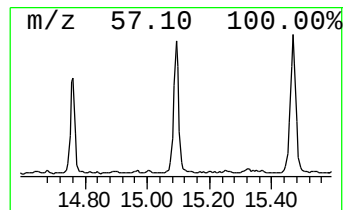
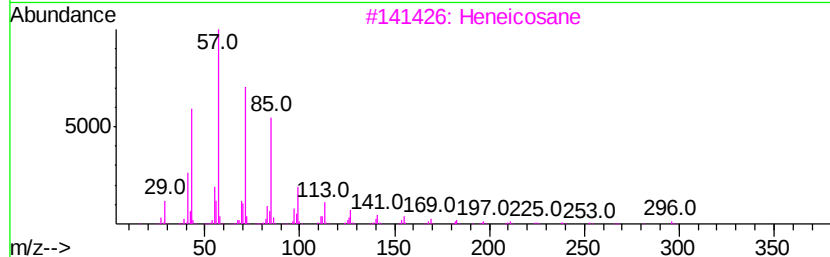
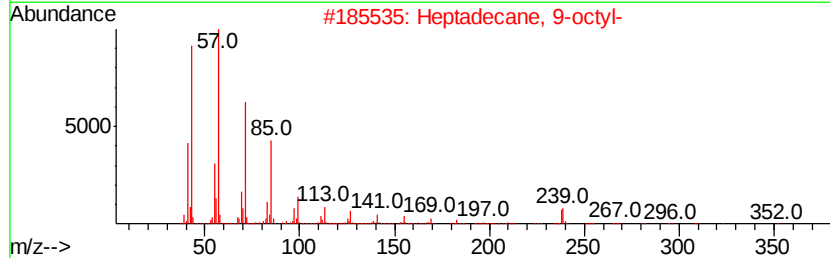
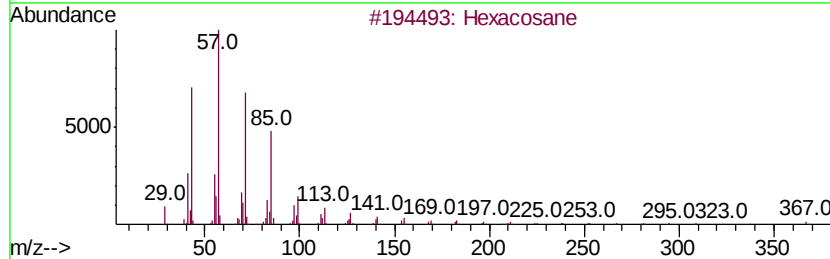
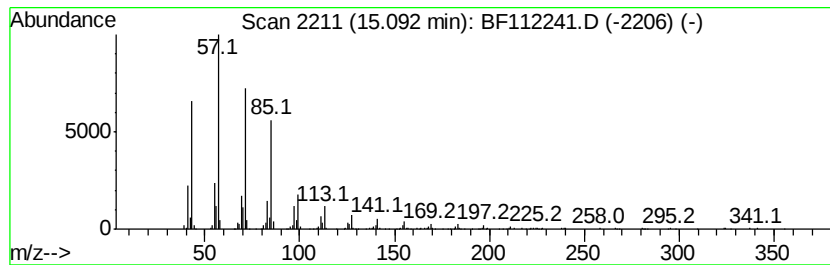
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	7.56 ng	696632	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012519\
Data File : BF112241.D
Acq On : 25 Jan 2019 19:32
Operator : JU/SJ
Sample : K1238-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

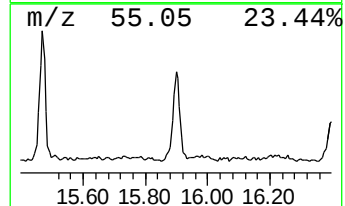
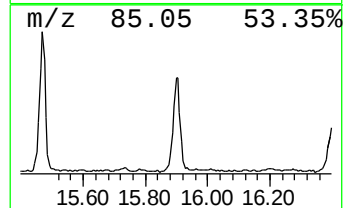
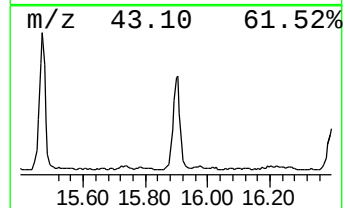
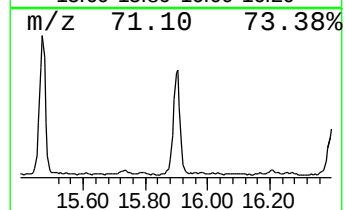
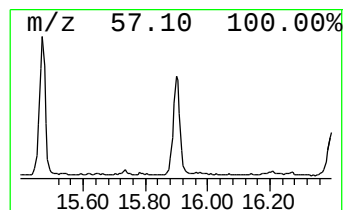
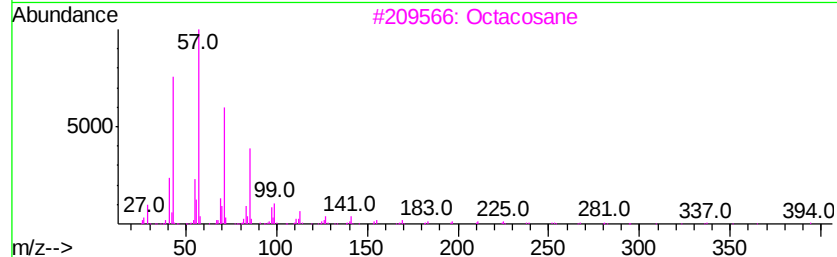
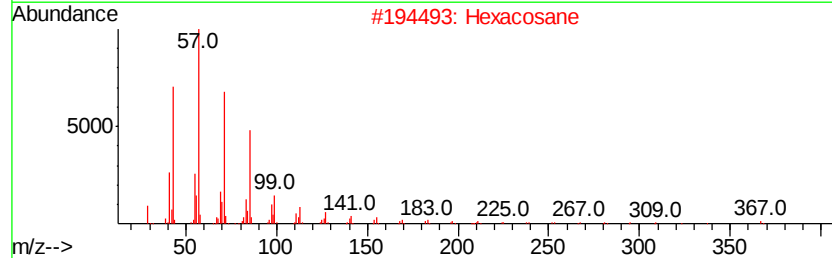
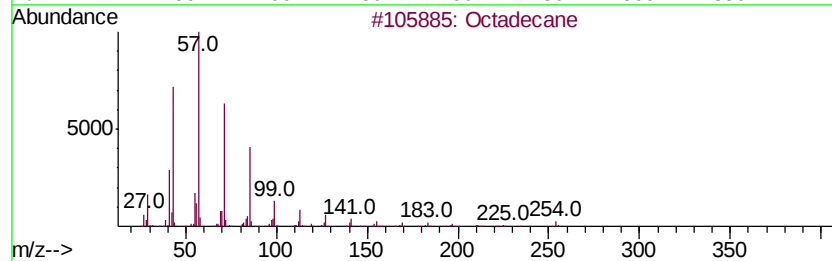
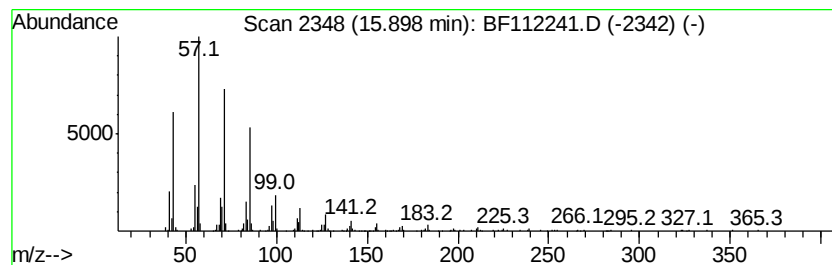
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	7.56 ng	696087	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Hexacosane	366	C26H54	000630-01-3	94
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012519\
Data File : BF112241.D
Acq On : 25 Jan 2019 19:32
Operator : JU/SJ
Sample : K1238-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

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
Butane, 2-methoxy...	2.16	3.7	ng	202231	1	6.84	1089060	20.0
2-Pentanone, 4-hy...	5.08	4.0	ng	220490	1	6.84	1089060	20.0
unknown6.62	6.62	97.5	ng	5310350	1	6.84	1089060	20.0
Phenol, 4,4'-(1-m...	12.83	17.8	ng	889625	5	14.00	998044	20.0
1-Decanol, 2-hexyl-	13.84	8.2	ng	409026	5	14.00	998044	20.0
Heneicosane	14.76	5.3	ng	487915	6	15.46	1842700	20.0
Hexacosane	15.09	7.6	ng	696632	6	15.46	1842700	20.0
Octadecane	15.90	7.6	ng	696087	6	15.46	1842700	20.0