

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102919\
 Data File : BF117606.D
 Acq On : 29 Oct 2019 23:00
 Operator : JU
 Sample : K5587-14
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CSA-2-1-10

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-BF101819.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	4.922	478	482	492	rBV	68207	100083	14.18%	1.607%
2	5.357	553	556	582	rBV	456793	637101	90.28%	10.228%
3	6.386	727	731	748	rBV	505622	685019	97.07%	10.998%
4	6.504	748	751	763	rVB	684075	705706	100.00%	11.330%
5	6.728	786	789	802	rVB	209538	188558	26.72%	3.027%
6	6.881	812	815	831	rBV	509067	518905	73.53%	8.331%
7	7.292	882	885	905	rBV	238565	357964	50.72%	5.747%
8	8.010	1004	1007	1018	rBV	149043	192910	27.34%	3.097%
9	9.080	1186	1189	1202	rBV	575427	582911	82.60%	9.358%
10	9.480	1254	1257	1271	rBB	64973	73427	10.40%	1.179%
11	9.763	1301	1305	1319	rBB	203155	199234	28.23%	3.199%
12	10.557	1437	1440	1456	rBV	264596	303316	42.98%	4.870%
13	11.251	1554	1558	1568	rBV	188387	208541	29.55%	3.348%
14	11.786	1646	1649	1656	rVV3	10816	17574	2.49%	0.282%
15	11.868	1660	1663	1664	rVV2	7357	7322	1.04%	0.118%
16	11.886	1664	1666	1670	rVB2	20450	16248	2.30%	0.261%
17	12.468	1762	1765	1769	rVB	52143	50854	7.21%	0.816%
18	12.698	1798	1804	1810	rBV	54799	65785	9.32%	1.056%
19	12.827	1822	1826	1833	rBV	618958	569676	80.72%	9.146%
20	12.910	1838	1840	1846	rVB4	5408	8177	1.16%	0.131%
21	13.027	1852	1860	1862	rBV3	7891	12741	1.81%	0.205%
22	13.133	1874	1878	1883	rVB2	6120	7255	1.03%	0.116%
23	13.392	1918	1922	1925	rBV3	8208	9963	1.41%	0.160%
24	13.680	1961	1971	1976	rBV5	20338	36403	5.16%	0.584%
25	13.745	1976	1982	1992	rVV6	26304	66405	9.41%	1.066%
26	13.857	1998	2001	2003	rBV	24665	20303	2.88%	0.326%
27	13.892	2003	2007	2011	rVV2	182244	214967	30.46%	3.451%
28	13.921	2011	2012	2016	rVB	30835	22575	3.20%	0.362%
29	13.974	2019	2021	2024	rVB3	7804	7872	1.12%	0.126%
30	14.039	2028	2032	2036	rVB2	14879	13716	1.94%	0.220%
31	14.345	2081	2084	2087	rVB	14889	14608	2.07%	0.235%
32	14.621	2128	2131	2132	rBV2	16470	15426	2.19%	0.248%
33	14.709	2143	2146	2150	rVB2	17008	18343	2.60%	0.294%
34	14.927	2179	2183	2185	rBV	22046	26957	3.82%	0.433%

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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	14.951	2185	2187	2193	rVB2	28933	35070	4.97%	0.563%
36	15.033	2199	2201	2206	rVB6	10435	11217	1.59%	0.180%
37	15.215	2229	2232	2237	rVB	13111	15209	2.16%	0.244%
38	15.280	2239	2243	2245	rVV2	12263	14420	2.04%	0.232%
39	15.333	2245	2252	2260	rVB	89661	131456	18.63%	2.110%
40	15.709	2312	2316	2321	rVB3	21818	32087	4.55%	0.515%
41	16.186	2393	2397	2401	rVB7	9088	12503	1.77%	0.201%

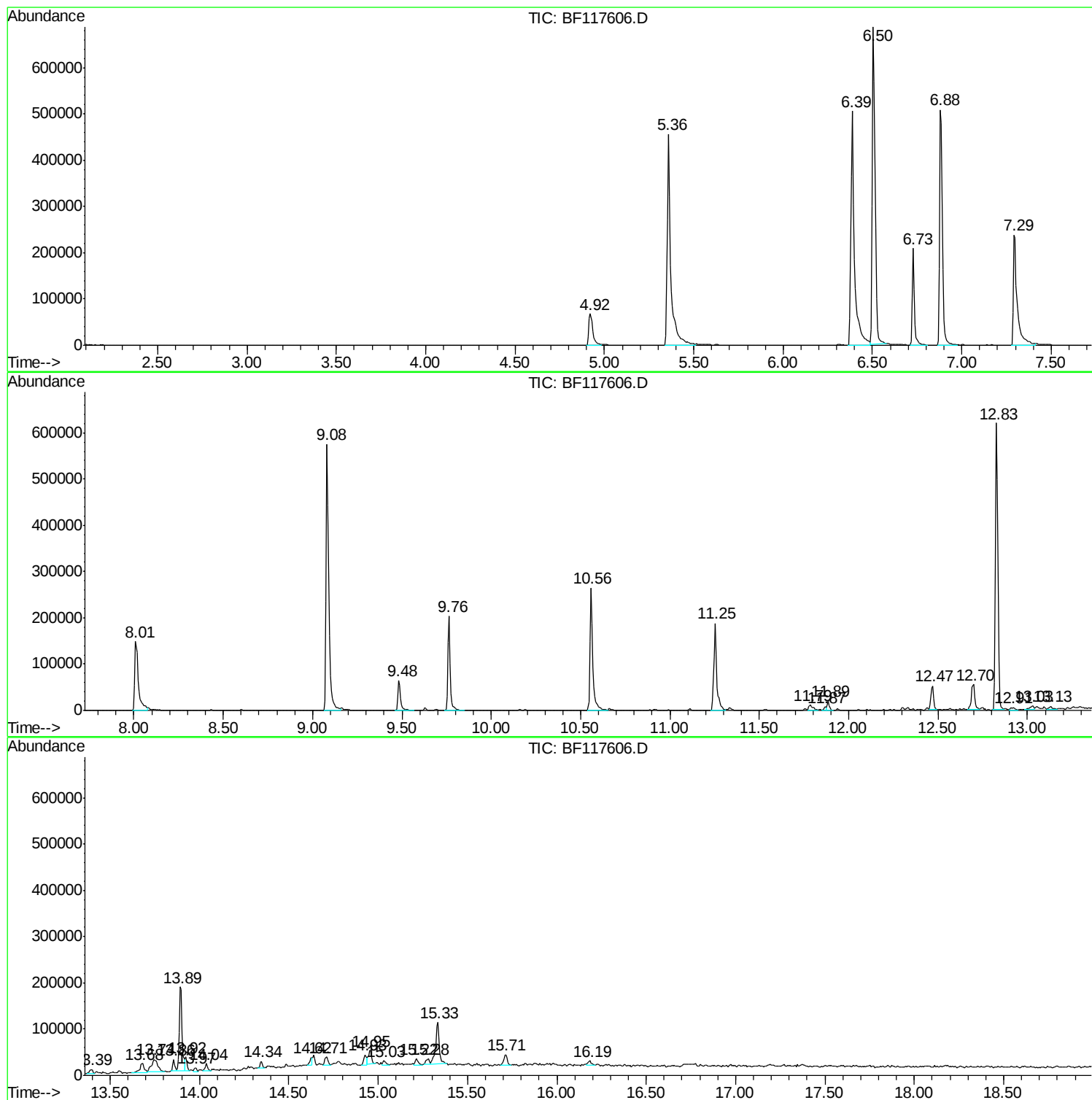
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Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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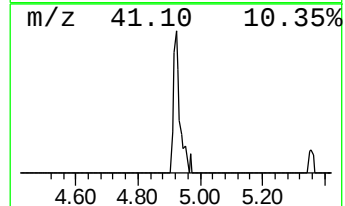
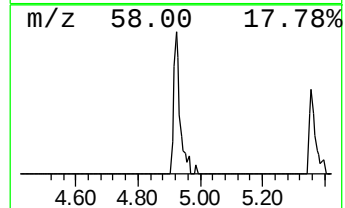
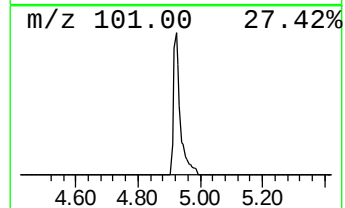
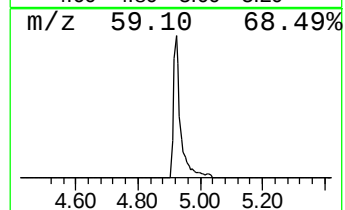
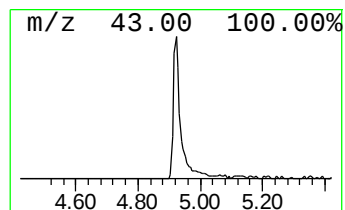
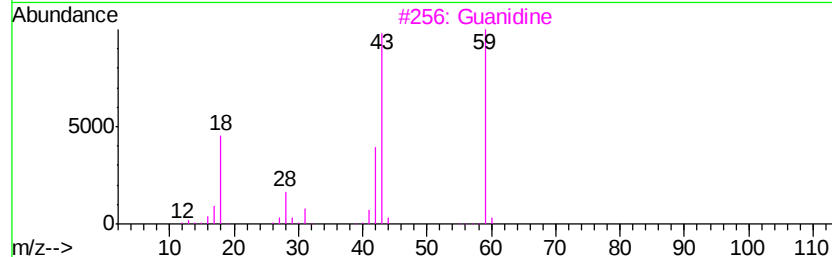
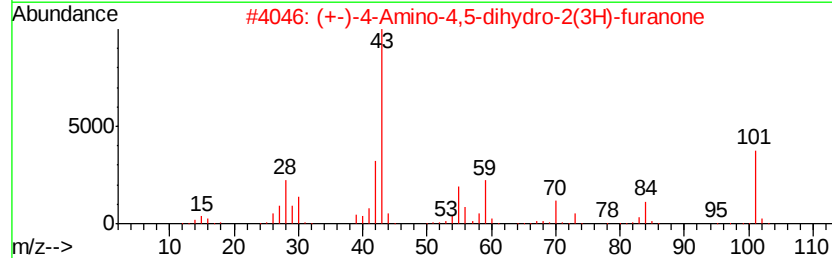
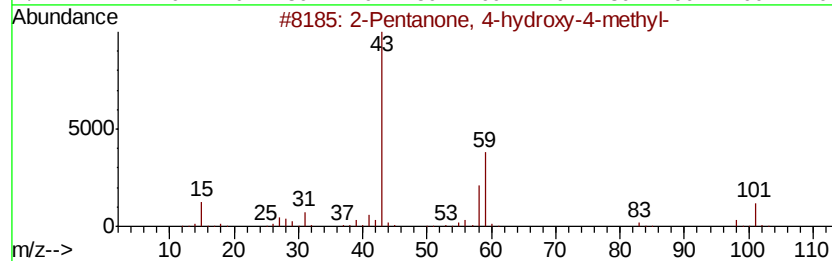
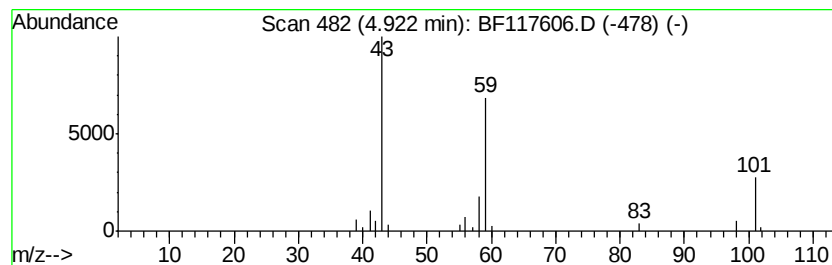
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	10.62 ng	100083	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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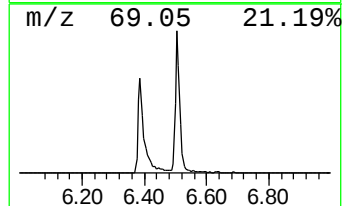
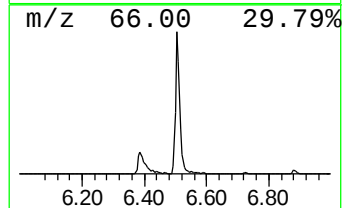
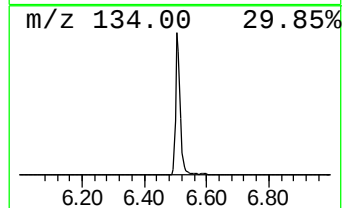
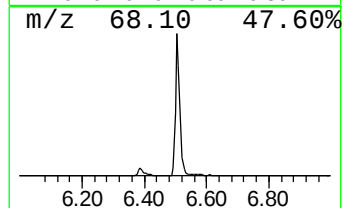
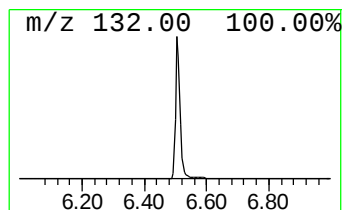
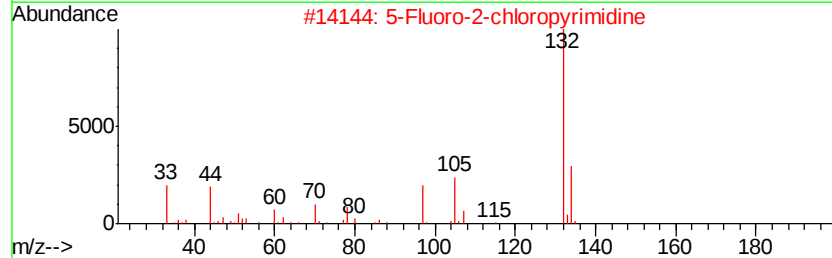
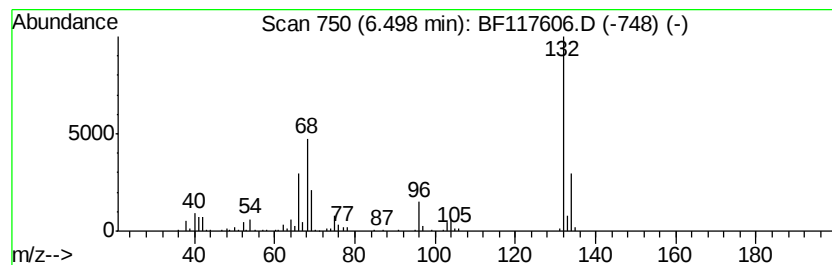
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	74.85 ng	705706	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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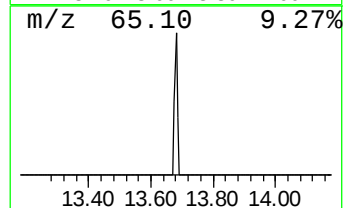
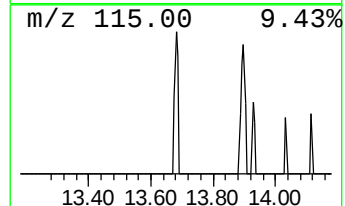
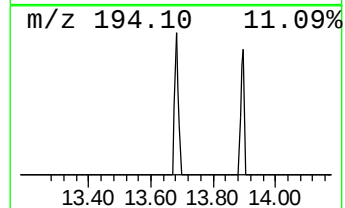
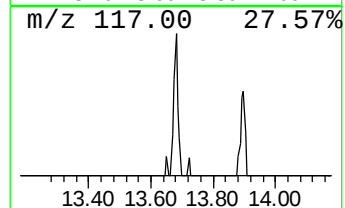
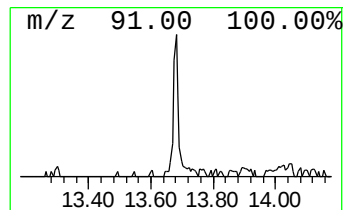
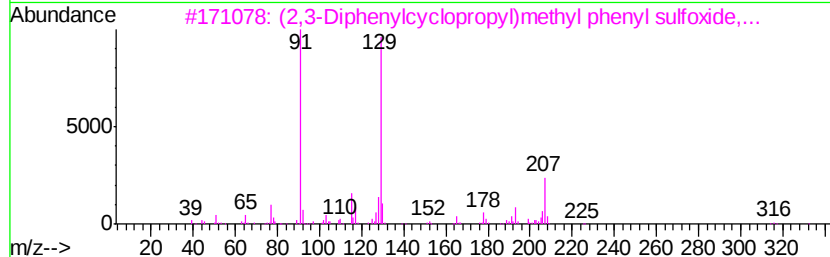
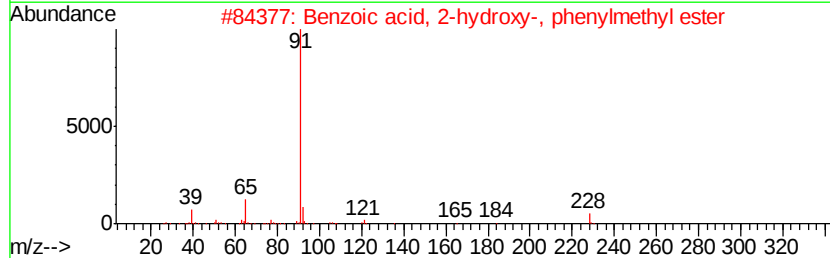
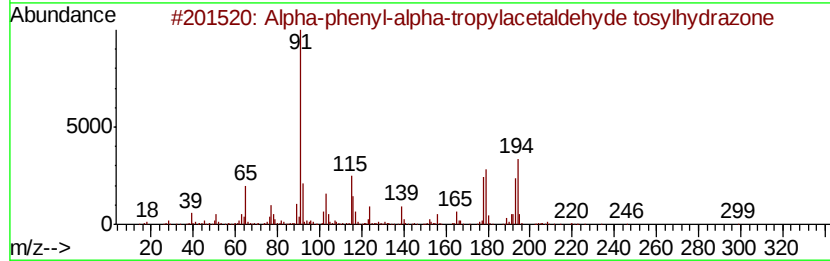
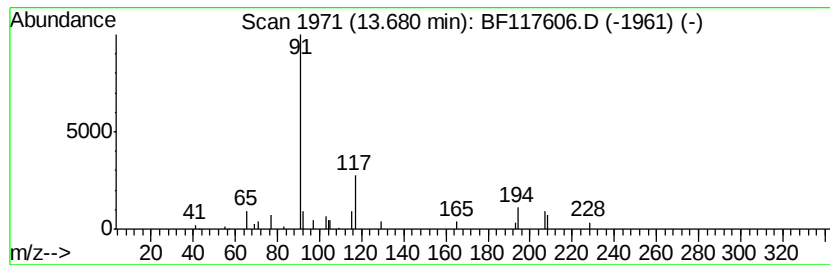
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown13.68 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.39 ng	36403	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Alpha-phenyl-alpha-trotylacetal...	378	C22H22N2O2S	022532-16-7	10
2		Benzoic acid, 2-hydroxy-, phenyl...	228	C14H12O3	000118-58-1	9
3		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O3	131758-71-9	9
4		Benzene, (4-bromobutyl)-	212	C10H13Br	013633-25-5	9
5		4-[Benzylamino]benzo-1,2,3-triazine	236	C14H12N4	026944-65-0	9



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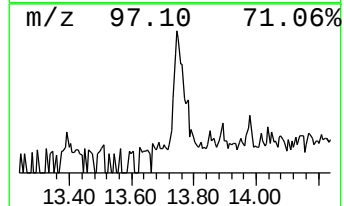
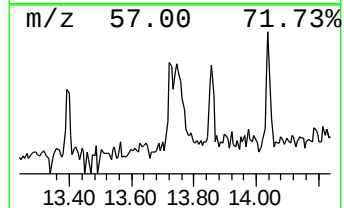
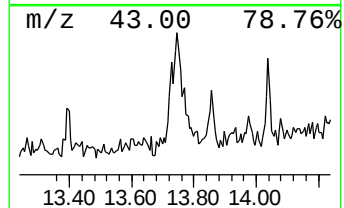
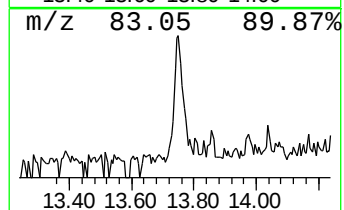
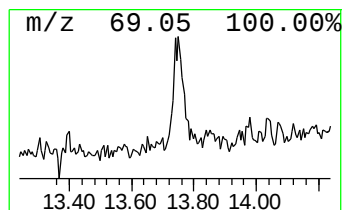
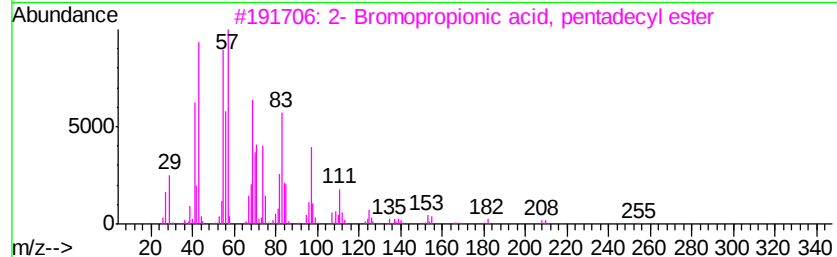
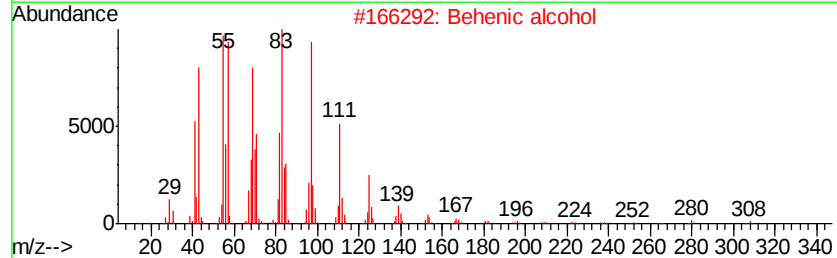
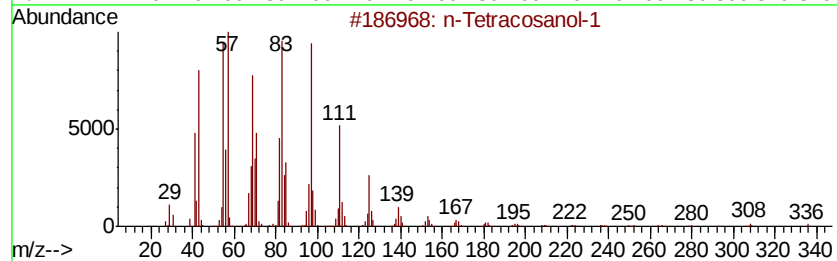
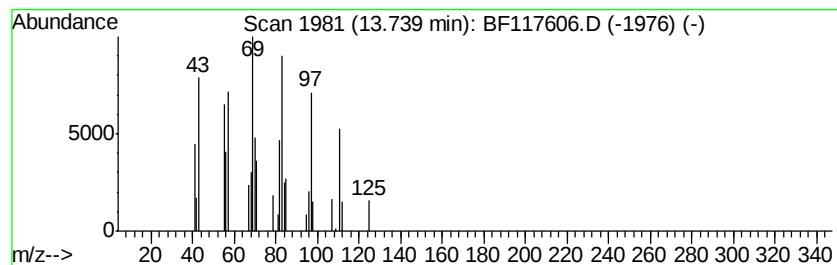
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	6.18 ng	66405	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	90
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
5		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	90



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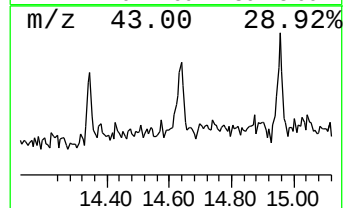
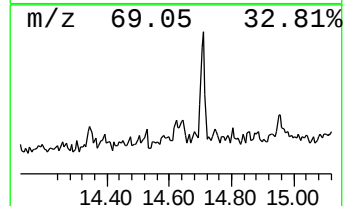
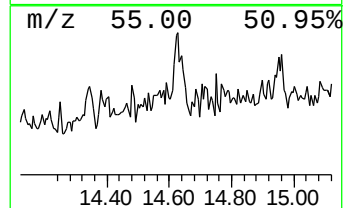
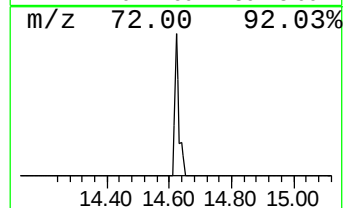
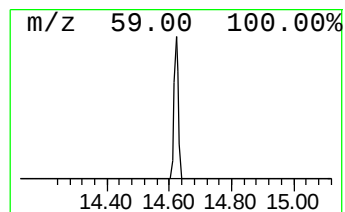
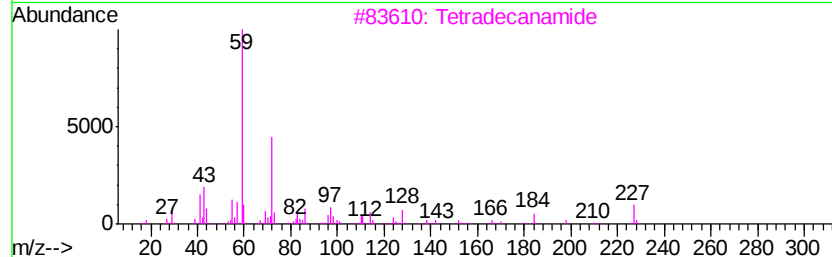
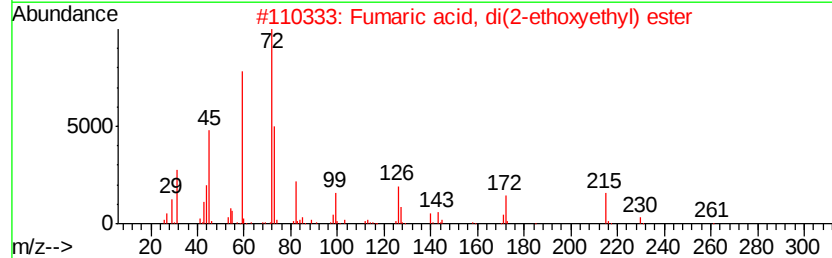
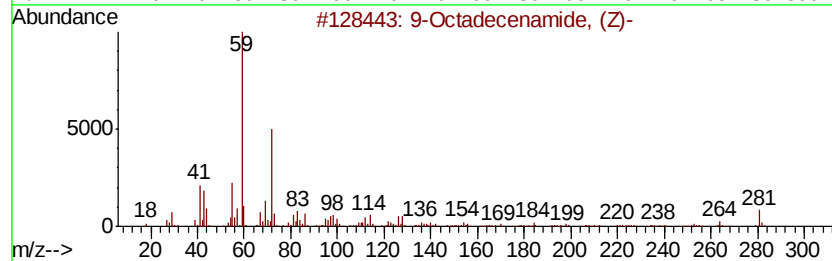
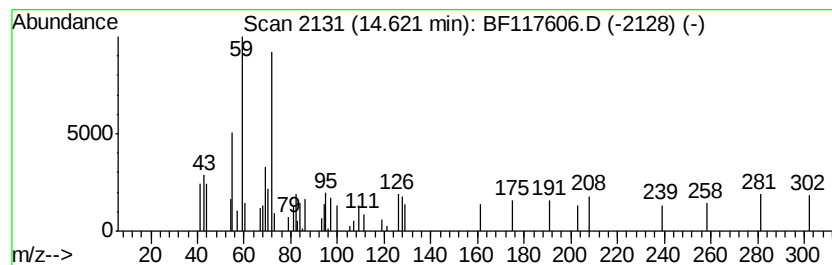
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.35 ng	15426	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
2		Fumaric acid, di(2-ethoxyethyl) ...	260	C12H20O6	1000330-57-5	38
3		Tetradecanamide	227	C14H29NO	000638-58-4	35
4		N-Isopropoxy-2-carbomethoxyvazeti...	173	C8H15NO3	053084-24-5	25
5		Octanamide	143	C8H17NO	000629-01-6	17



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117606.D
Acq On : 29 Oct 2019 23:00
Operator : JU
Sample : K5587-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSA-2-1-10

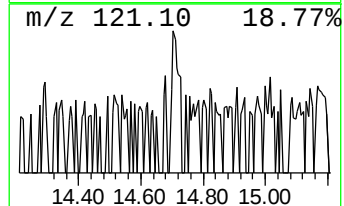
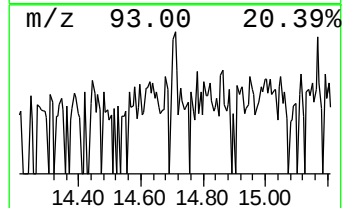
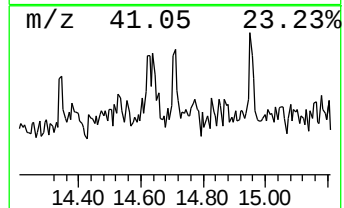
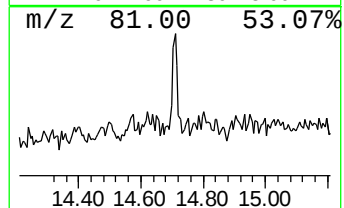
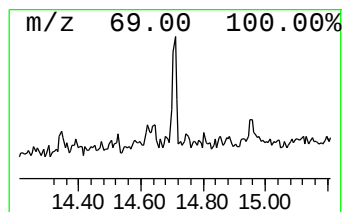
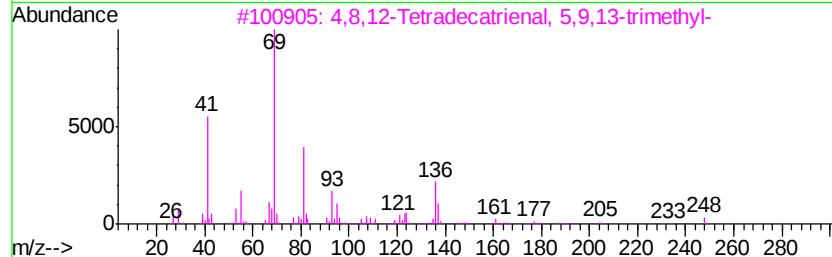
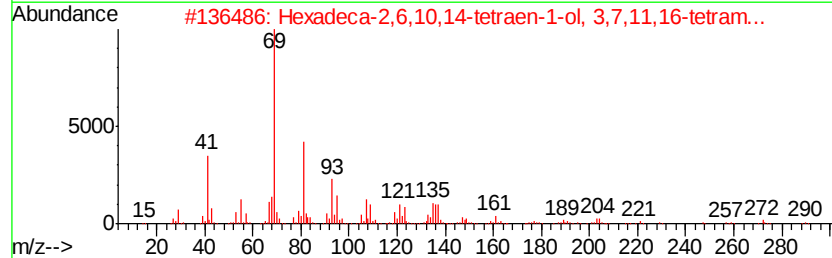
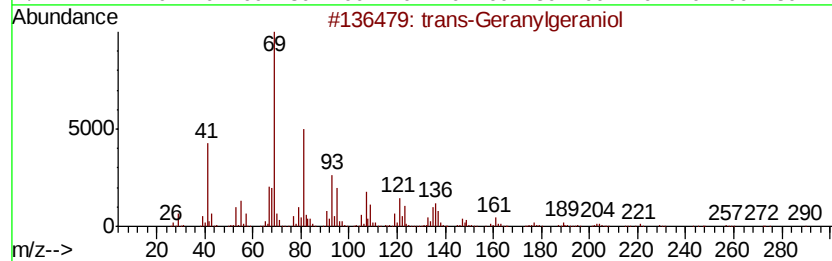
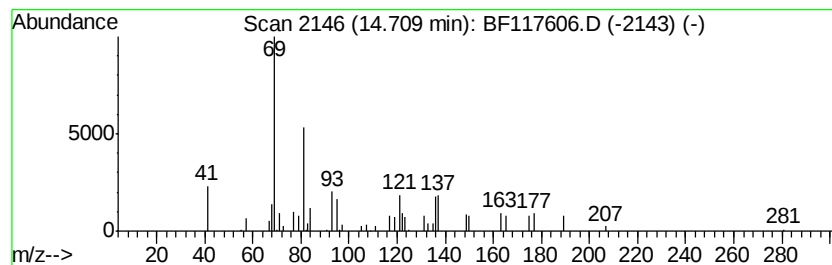
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 trans-Geranylgeraniol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.79 ng	18343	Perylene-d12	15.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Geranylgeraniol	290	C20H34O	024034-73-9	64
2			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	59
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
4			Farnesol isomer a	222	C15H26O	1000108-92-4	56
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
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Sample : K5587-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSA-2-1-10

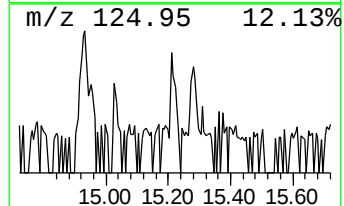
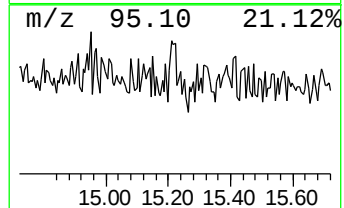
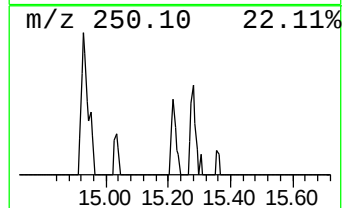
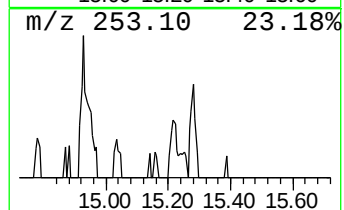
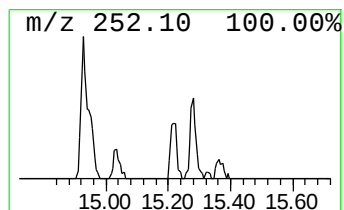
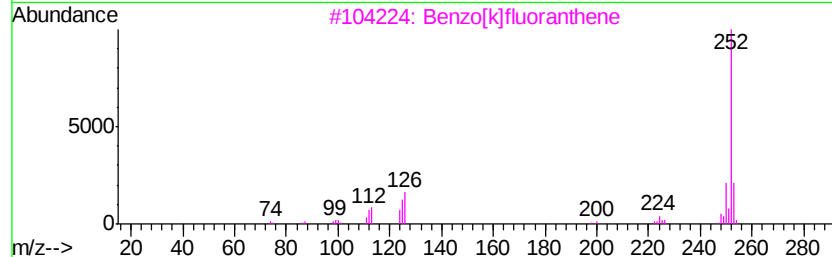
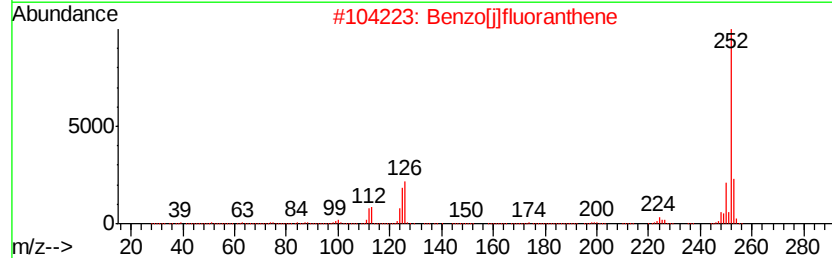
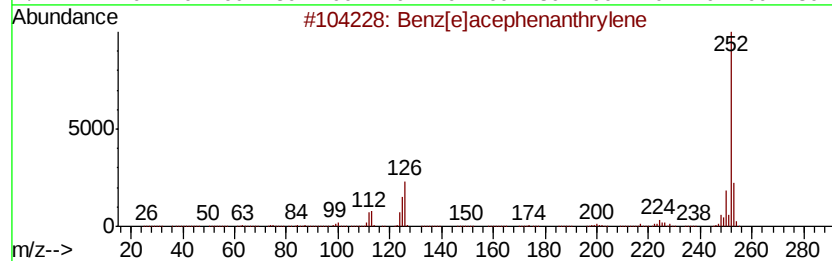
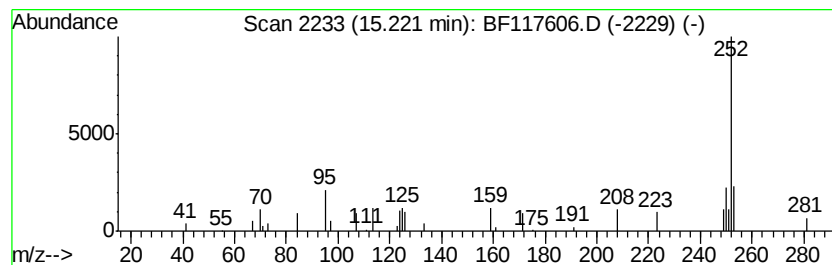
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.31 ng	15209	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	49
2		Benzo[i]fluoranthene	252	C20H12	000205-82-3	49
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	49
4		Perylene	252	C20H12	000198-55-0	49
5		Benzo[e]pyrene	252	C20H12	000192-97-2	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
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Acq On : 29 Oct 2019 23:00
Operator : JU
Sample : K5587-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSA-2-1-10

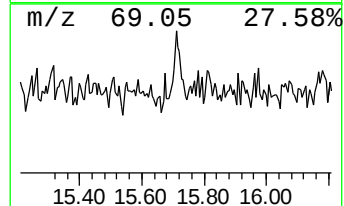
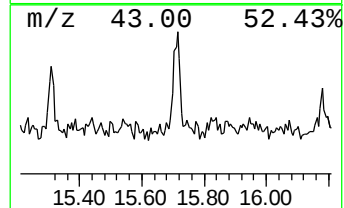
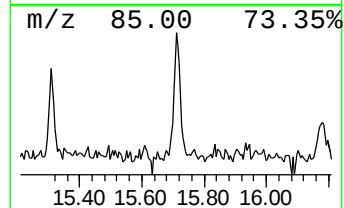
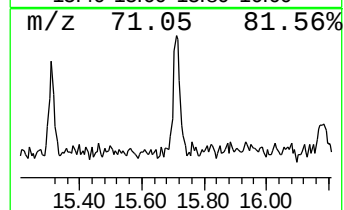
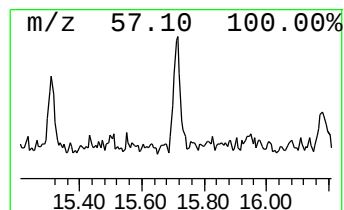
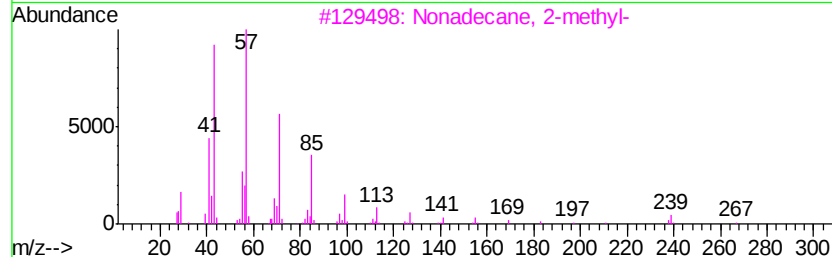
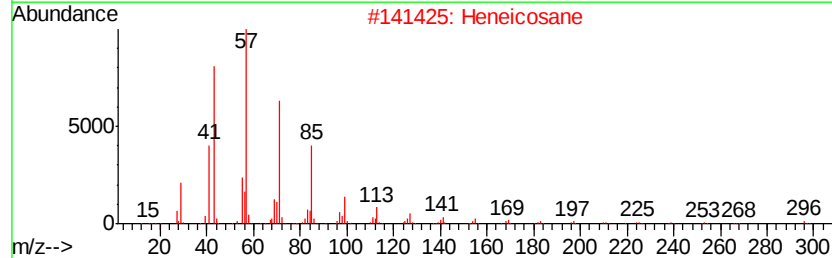
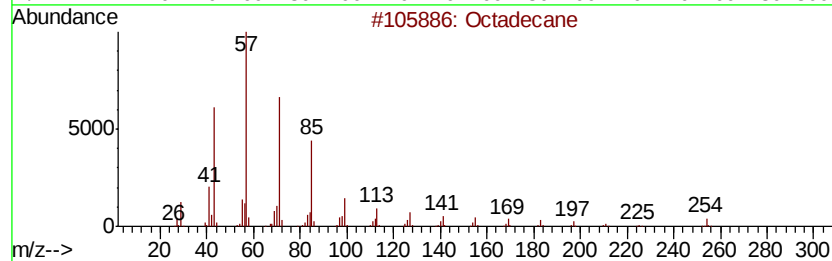
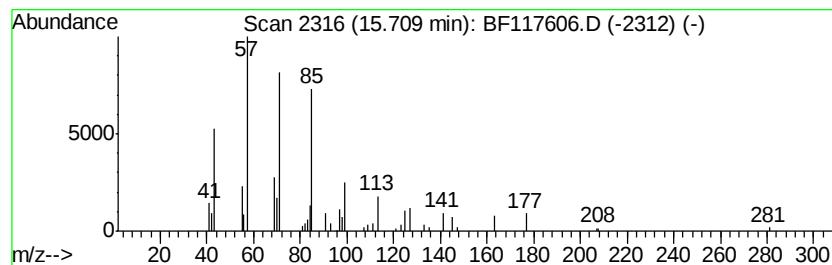
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	4.88 ng	32087	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	78
2	Heneicosane	296	C21H44	000629-94-7	78
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Docosane	310	C22H46	000629-97-0	78



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Operator : JU
Sample : K5587-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CSA-2-1-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
2-Pentanone, 4-hy...	4.92	10.6	ng	100083	1	6.73	188558	20.0
unknown6.50	6.50	74.8	ng	705706	1	6.73	188558	20.0
unknown13.68	13.68	3.4	ng	36403	5	13.90	214967	20.0
n-Tetracosanol-1	13.74	6.2	ng	66405	5	13.90	214967	20.0
9-Octadecenamide,...	14.62	2.4	ng	15426	6	15.33	131456	20.0
trans-Geranylgera...	14.71	2.8	ng	18343	6	15.33	131456	20.0
Perylene	15.22	2.3	ng	15209	6	15.33	131456	20.0
Octadecane	15.71	4.9	ng	32087	6	15.33	131456	20.0