

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
 Data File : BF118331.D
 Acq On : 26 Dec 2019 22:08
 Operator : JU
 Sample : K6436-06 2X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K009-WC-1

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-BF122419.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	5.040	498	502	514	rVB	114727	129101	12.04%	0.941%
2	5.463	570	574	584	rBV	644929	679817	63.39%	4.957%
3	6.481	744	747	762	rBV	806356	814454	75.94%	5.939%
4	6.622	767	771	779	rBV	941675	863727	80.54%	6.298%
5	6.851	806	810	816	rBV	878935	694672	64.77%	5.066%
6	7.004	833	836	845	rBV	782963	696166	64.91%	5.076%
7	7.416	902	906	917	rBV	421424	463823	43.25%	3.382%
8	8.139	1025	1029	1035	rBV	1061470	906646	84.54%	6.611%
9	9.216	1208	1212	1221	rBV	1274291	1072465	100.00%	7.820%
10	9.292	1222	1225	1228	rVB3	16488	16133	1.50%	0.118%
11	9.486	1249	1258	1261	rBV6	21419	33797	3.15%	0.246%
12	9.557	1267	1270	1272	rBV	17224	18882	1.76%	0.138%
13	9.610	1276	1279	1282	rVV	53787	53457	4.98%	0.390%
14	9.757	1302	1304	1310	rBV3	16089	20309	1.89%	0.148%
15	9.898	1323	1328	1332	rBV	1247257	1041213	97.09%	7.592%
16	9.933	1332	1334	1337	rVB	20248	17212	1.60%	0.126%
17	10.004	1342	1346	1351	rBV7	13552	18289	1.71%	0.133%
18	10.104	1360	1363	1367	rVB3	18944	20256	1.89%	0.148%
19	10.145	1367	1370	1373	rBV3	17650	17685	1.65%	0.129%
20	10.216	1379	1382	1384	rBV3	23988	23166	2.16%	0.169%
21	10.310	1393	1398	1399	rBV5	14526	17460	1.63%	0.127%
22	10.322	1399	1400	1404	rVB2	22248	18067	1.68%	0.132%
23	10.692	1460	1463	1473	rBV	478126	453877	42.32%	3.310%
24	10.810	1478	1483	1487	rBV3	41490	63188	5.89%	0.461%
25	10.963	1505	1509	1512	rBV6	8268	14776	1.38%	0.108%
26	11.251	1555	1558	1560	rBV	25846	24359	2.27%	0.178%
27	11.280	1560	1563	1569	rVB4	36018	55227	5.15%	0.403%
28	11.392	1578	1582	1585	rBV	1081411	929276	86.65%	6.776%
29	11.416	1585	1586	1588	rVB	71638	41032	3.83%	0.299%
30	11.469	1593	1595	1598	rVB	19531	18792	1.75%	0.137%
31	11.675	1628	1630	1635	rVB2	32878	32776	3.06%	0.239%
32	11.727	1636	1639	1644	rVV3	21207	25953	2.42%	0.189%
33	11.916	1668	1671	1679	rVB5	95454	127911	11.93%	0.933%
34	12.004	1684	1686	1689	rVV2	27510	29608	2.76%	0.216%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122619\
 Data File : BF118331.D
 Acq On : 26 Dec 2019 22:08
 Operator : JU
 Sample : K6436-06 2X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K009-WC-1

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-BF122419.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.033	1689	1691	1695	rVB	26248	20341	1.90%	0.148%
36	12.086	1697	1700	1705	rBV2	43846	40501	3.78%	0.295%
37	12.127	1705	1707	1710	rBV3	22682	23666	2.21%	0.173%
38	12.192	1716	1718	1720	rBV2	18653	16944	1.58%	0.124%
39	12.322	1738	1740	1746	rBV5	31859	49047	4.57%	0.358%
40	12.374	1746	1749	1751	rBV3	29451	35024	3.27%	0.255%
41	12.451	1758	1762	1764	rBV2	46444	57095	5.32%	0.416%
42	12.475	1764	1766	1770	rVV4	64773	66423	6.19%	0.484%
43	12.504	1770	1771	1774	rVV2	22237	18813	1.75%	0.137%
44	12.610	1786	1789	1795	rBV	244515	306337	28.56%	2.234%
45	12.710	1803	1806	1809	rBV4	51518	66772	6.23%	0.487%
46	12.845	1823	1829	1835	rBV	238214	332857	31.04%	2.427%
47	12.898	1836	1838	1842	rVV3	41143	38690	3.61%	0.282%
48	12.980	1848	1852	1855	rBV	1212822	948741	88.46%	6.918%
49	13.204	1888	1890	1894	rBV2	62547	74290	6.93%	0.542%
50	13.551	1947	1949	1952	rBV2	83889	77865	7.26%	0.568%
51	13.880	2002	2005	2011	rVB2	162496	194892	18.17%	1.421%
52	14.045	2030	2033	2036	rBV	910140	933160	87.01%	6.805%
53	14.198	2057	2059	2061	rBV	125779	102785	9.58%	0.750%
54	15.539	2284	2287	2294	rVB2	645667	855970	79.81%	6.242%

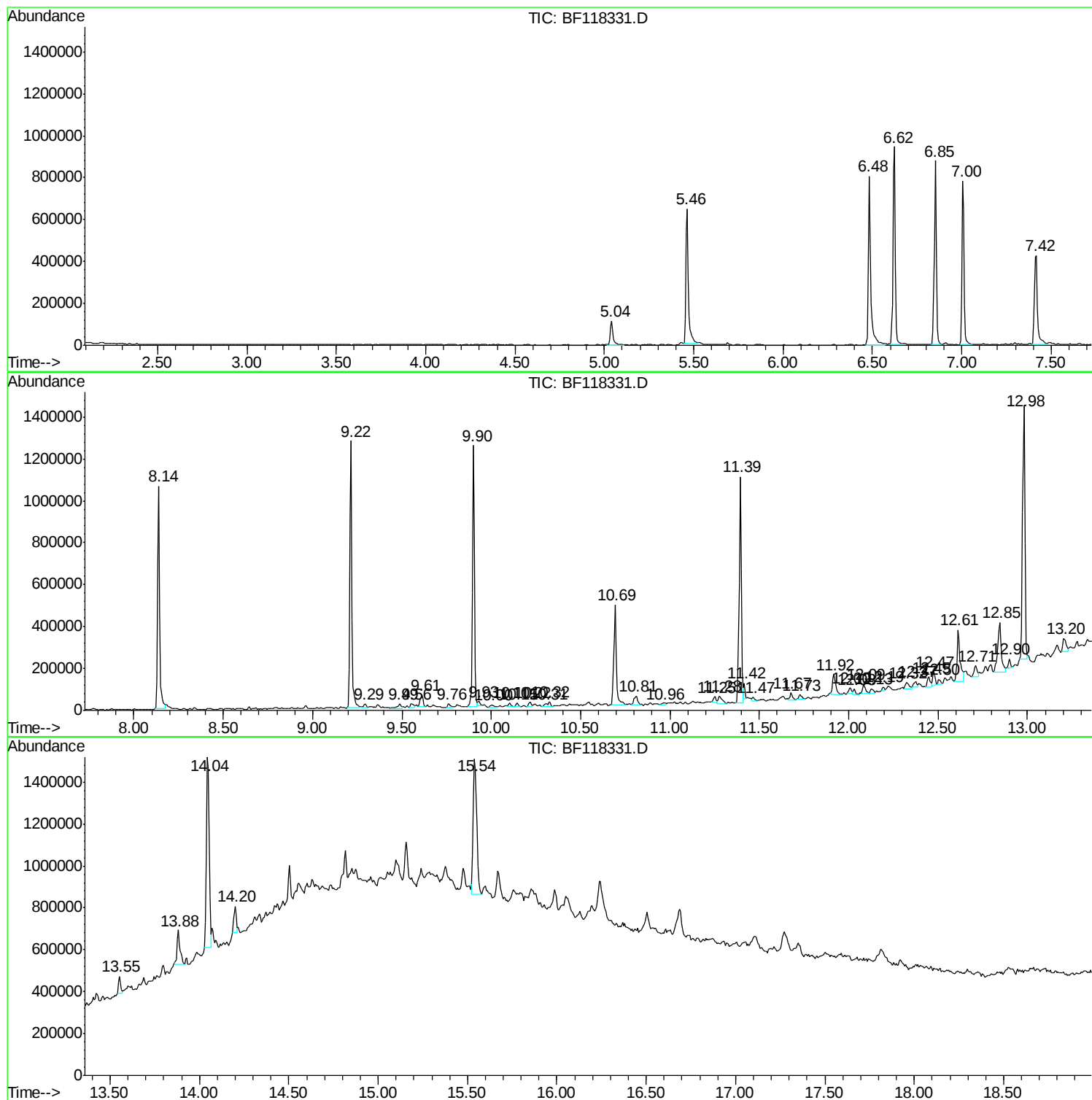
Sum of corrected areas: 13713785

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

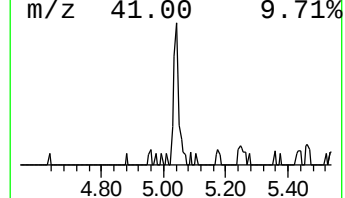
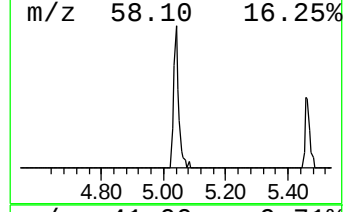
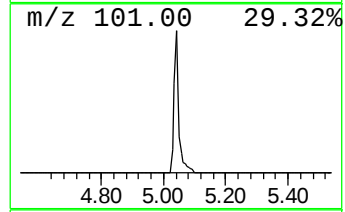
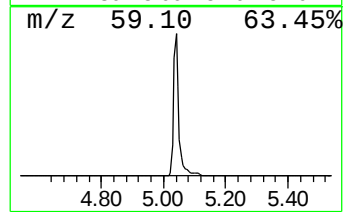
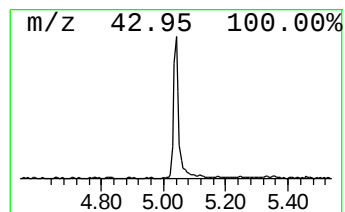
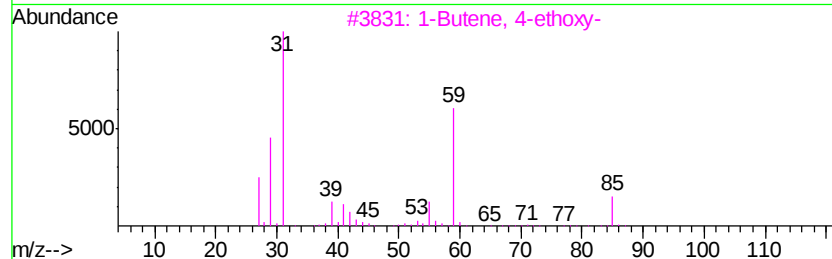
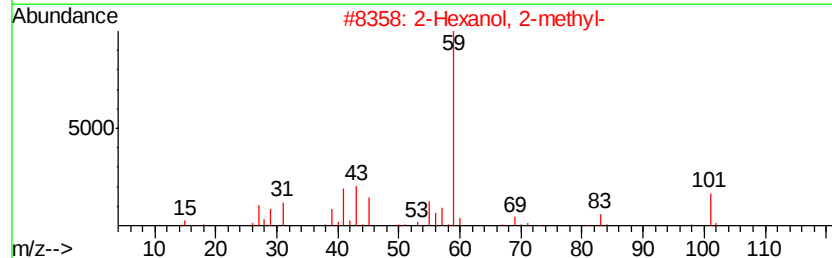
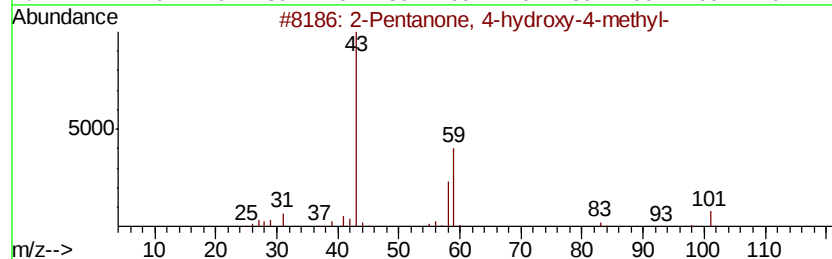
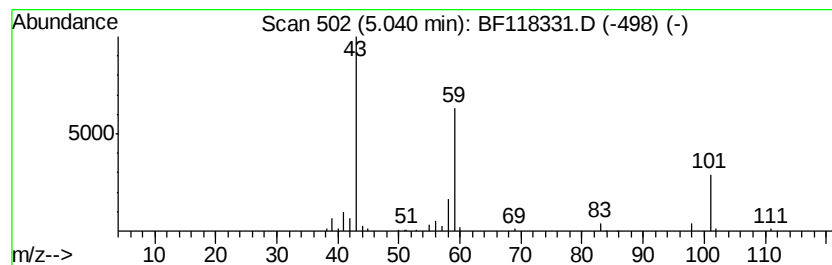
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	3.72 ng	129101	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

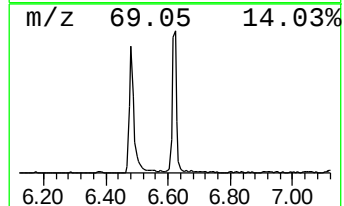
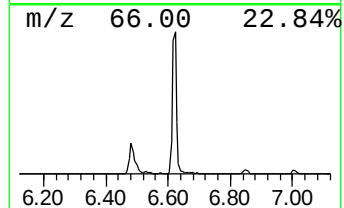
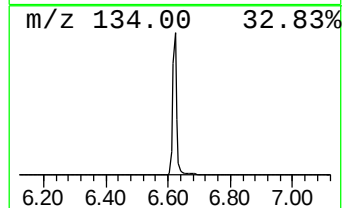
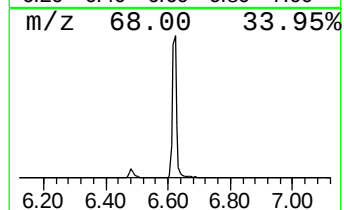
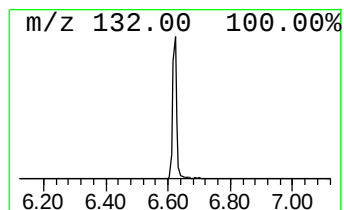
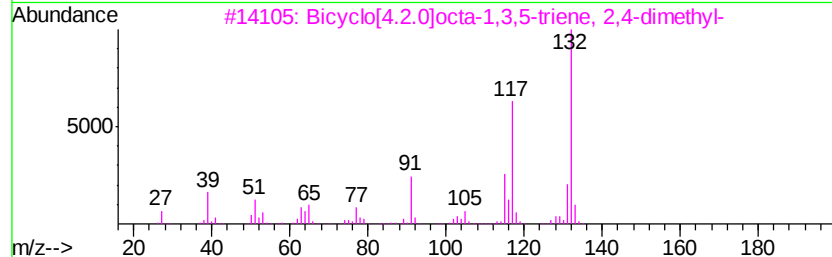
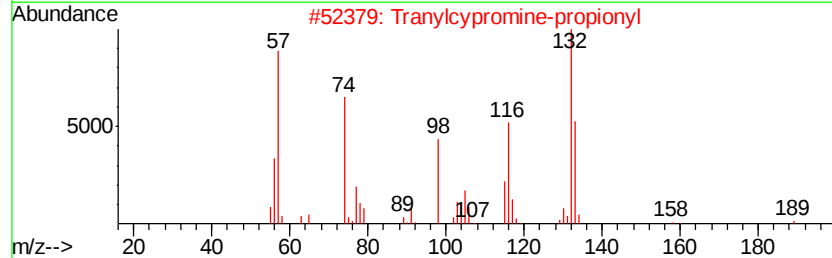
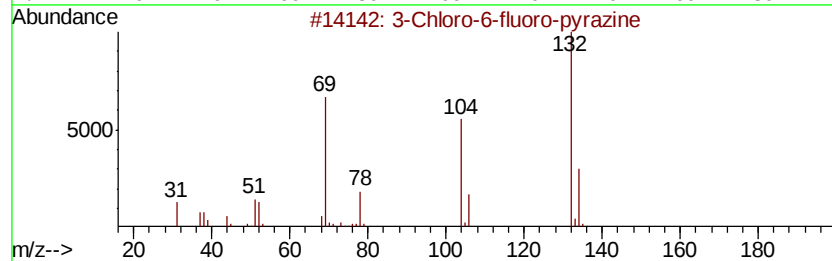
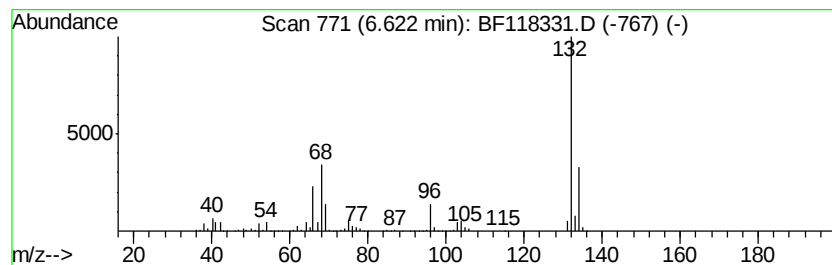
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	24.87 ng	863727	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

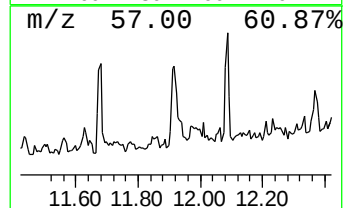
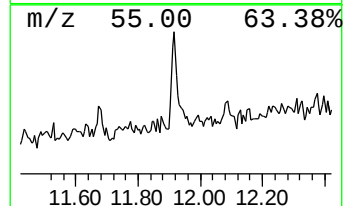
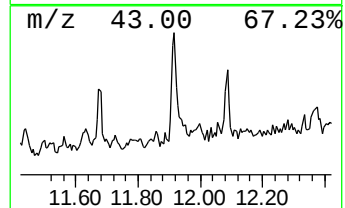
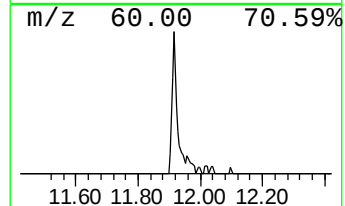
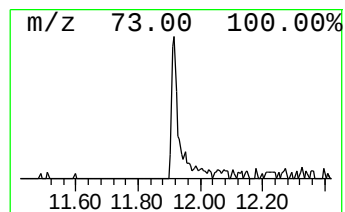
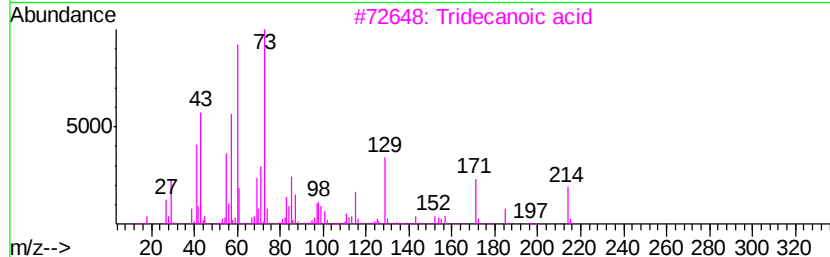
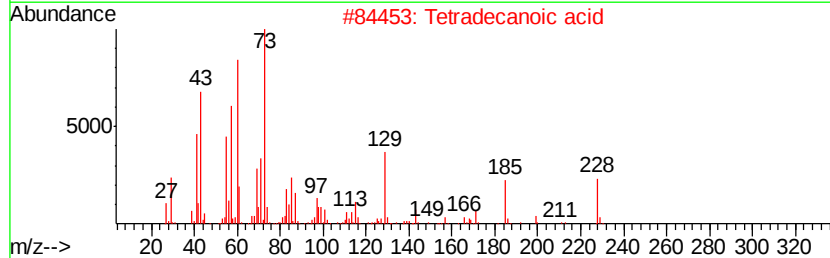
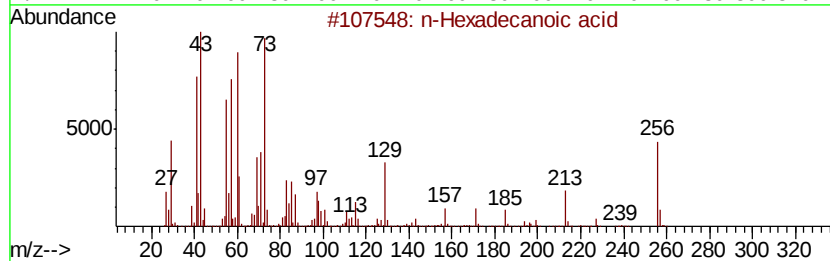
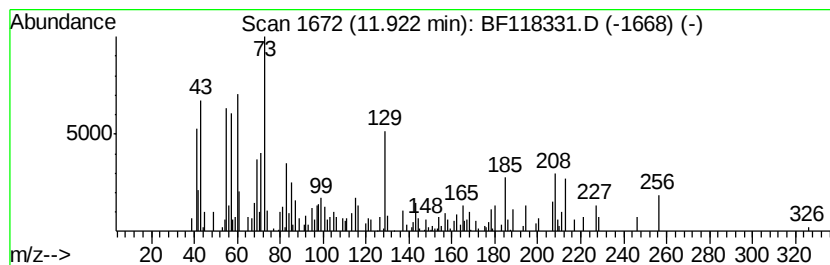
Instrument :
BNA_F
ClientSampleId :
K009-WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	2.75 ng	127911	Phenanthrene-d10	11.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Octadecanoic acid	284	C18H36O2	000057-11-4	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

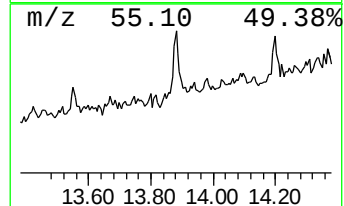
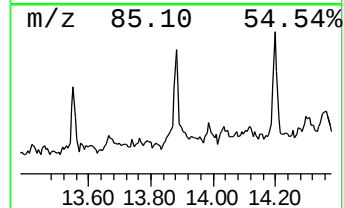
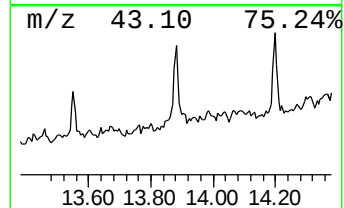
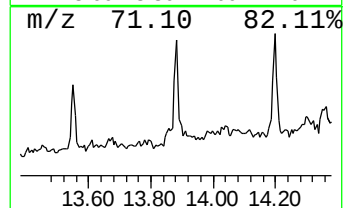
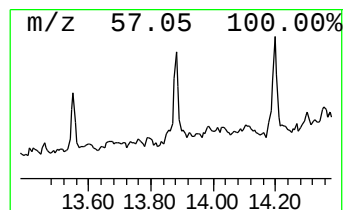
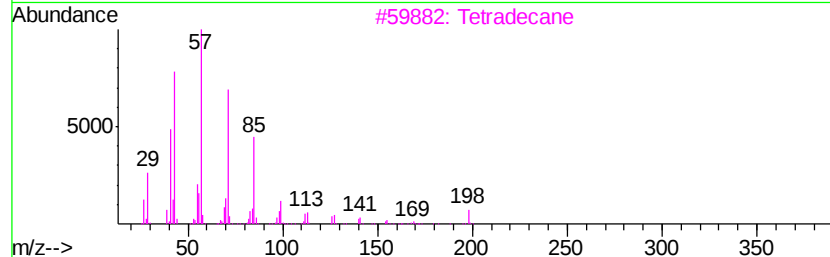
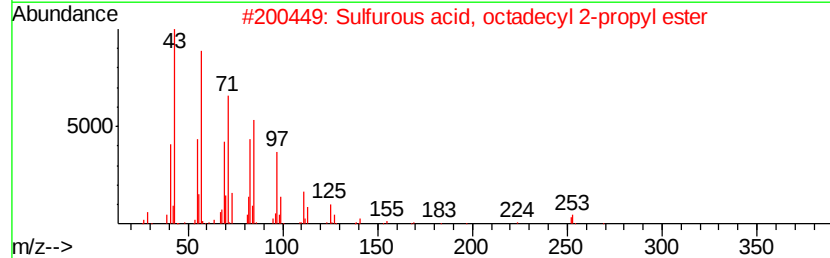
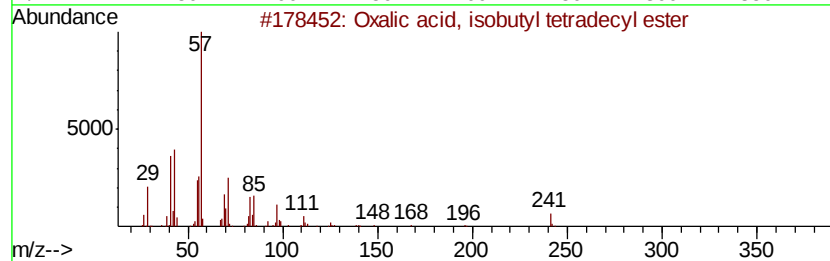
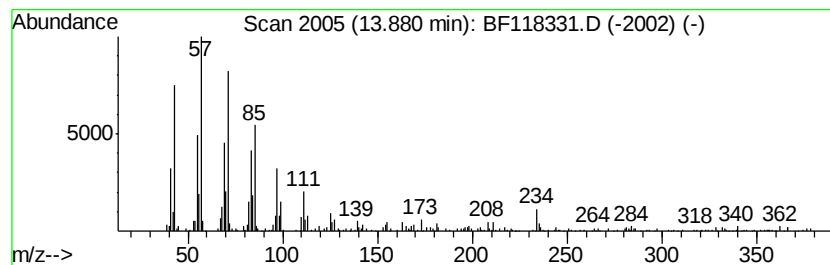
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Oxalic acid, isobutyl tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	4.18 ng	194892	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	86
2		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	81
3		Tetradecane	198	C14H30	000629-59-4	70
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	64
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

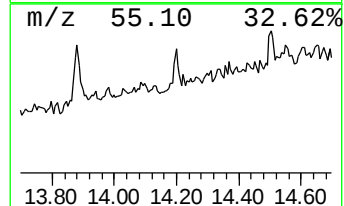
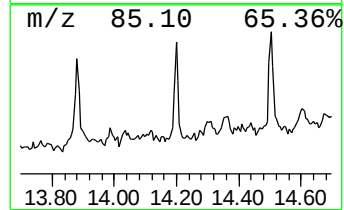
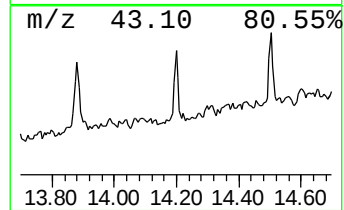
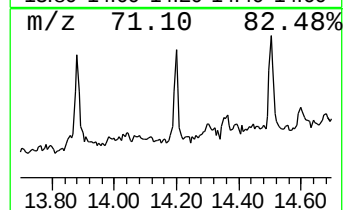
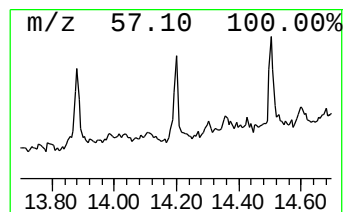
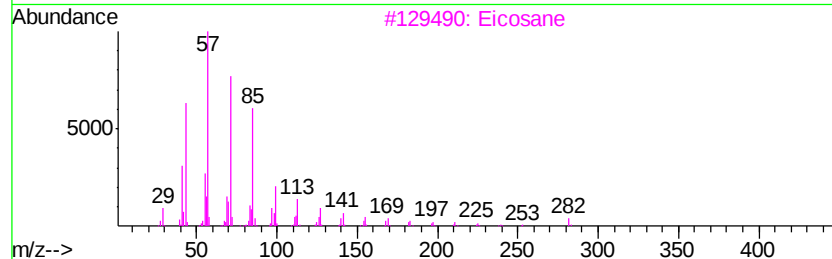
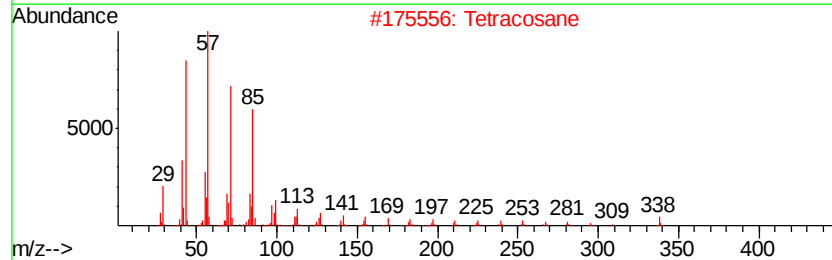
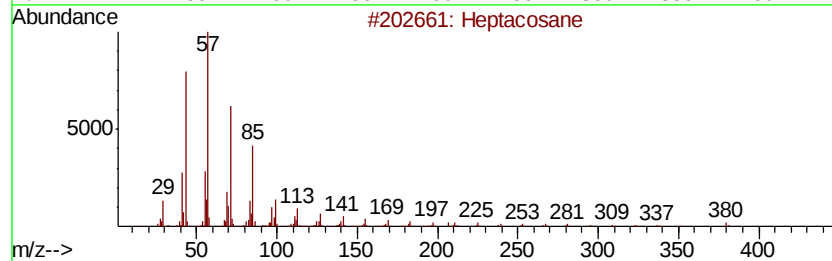
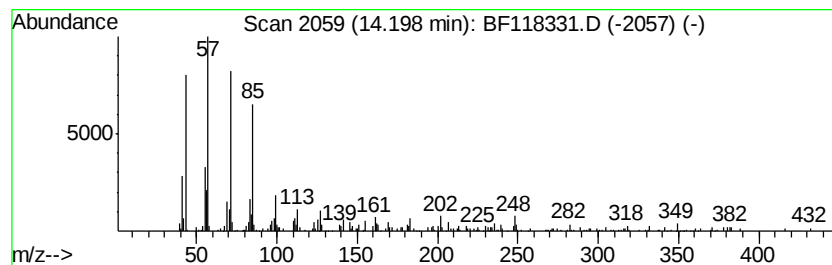
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	2.20 ng	102785	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	93
2	Tetracosane		338	C24H50	000646-31-1	90
3	Eicosane		282	C20H42	000112-95-8	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Pentadecane, 4-methyl-		226	C16H34	002801-87-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122619\
Data File : BF118331.D
Acq On : 26 Dec 2019 22:08
Operator : JU
Sample : K6436-06 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K009-WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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...	5.04	3.7	ng	129101	1	6.85	694672	20.0
unknown6.62	6.62	24.9	ng	863727	1	6.85	694672	20.0
n-Hexadecanoic acid	11.92	2.8	ng	127911	4	11.39	929276	20.0
Oxalic acid, isob...	13.88	4.2	ng	194892	5	14.05	933160	20.0
Heptacosane	14.20	2.2	ng	102785	5	14.05	933160	20.0