

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010319\
 Data File : BF111840.D
 Acq On : 4 Jan 2019 00:00
 Operator : JU/SJ
 Sample : K1019-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEST-PIT-D-11-12-A

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-BF121918.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	2.210	16	21	26	rVB	104951	145625	2.38%	0.306%
2	3.446	228	231	239	rBV	78232	146892	2.40%	0.308%
3	5.128	510	517	525	rBV	243994	320459	5.24%	0.673%
4	5.540	582	587	590	rBV	4912197	5009771	81.99%	10.514%
5	6.545	753	758	763	rBV	4786270	5685647	93.05%	11.932%
6	6.681	776	781	784	rBV	5767855	5311718	86.93%	11.147%
7	6.904	815	819	822	rBV	1727898	1422984	23.29%	2.986%
8	7.063	841	846	849	rBV	4815594	4211102	68.92%	8.838%
9	7.463	909	914	917	rBV	3666151	3324625	54.41%	6.977%
10	8.187	1033	1037	1040	rBV	2207229	1771853	29.00%	3.718%
11	9.257	1215	1219	1223	rBV	6360267	6110035	100.00%	12.823%
12	9.645	1281	1285	1290	rBV	816593	654847	10.72%	1.374%
13	9.939	1331	1335	1339	rBV2	2161681	1826924	29.90%	3.834%
14	10.728	1465	1469	1477	rBV	2690463	2401642	39.31%	5.040%
15	11.427	1584	1588	1590	rBV	1590425	1356851	22.21%	2.848%
16	11.451	1590	1592	1595	rVV	408804	338125	5.53%	0.710%
17	11.498	1598	1600	1603	rVB	114641	92689	1.52%	0.195%
18	11.927	1667	1673	1675	rBV	58401	62513	1.02%	0.131%
19	11.957	1675	1678	1683	rVB	80975	81475	1.33%	0.171%
20	12.039	1689	1692	1695	rBV	84355	99155	1.62%	0.208%
21	12.639	1791	1794	1798	rVB	508201	425370	6.96%	0.893%
22	12.869	1827	1833	1839	rBV	407266	438958	7.18%	0.921%
23	13.010	1850	1857	1860	rBV	3878417	3365275	55.08%	7.062%
24	13.904	2006	2009	2014	rVB2	148178	188007	3.08%	0.395%
25	14.069	2032	2037	2039	rBV2	1324235	1484776	24.30%	3.116%
26	14.092	2039	2041	2046	rVB	208000	184385	3.02%	0.387%
27	14.221	2061	2063	2067	rBV	63360	61182	1.00%	0.128%
28	14.839	2166	2168	2173	rVB	69674	63968	1.05%	0.134%
29	15.115	2212	2215	2222	rVB	86291	151172	2.47%	0.317%
30	15.186	2225	2227	2231	rVB2	64656	64916	1.06%	0.136%
31	15.486	2276	2278	2281	rVB	67548	64682	1.06%	0.136%
32	15.557	2285	2290	2301	rVB	509143	782563	12.81%	1.642%

LSC Area Percent Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TEST-PIT-D-11-12-A

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-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

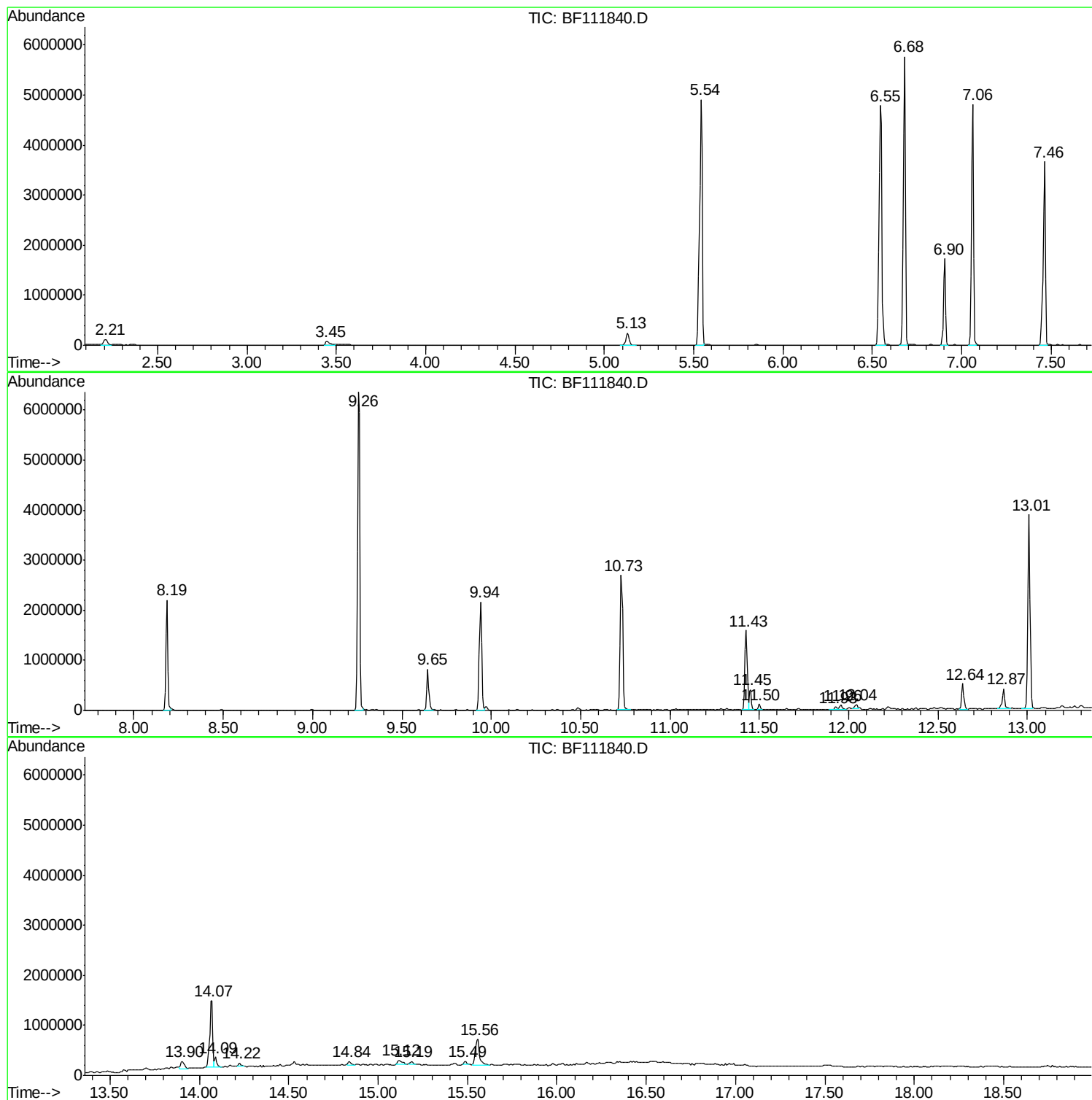
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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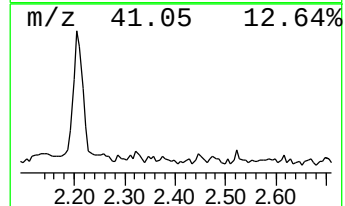
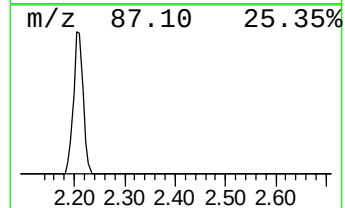
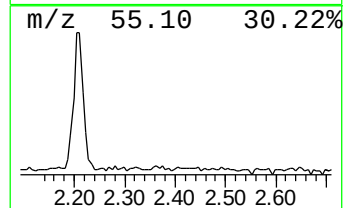
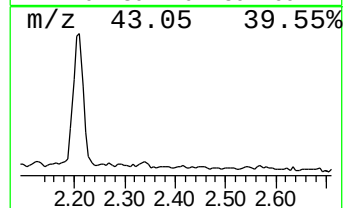
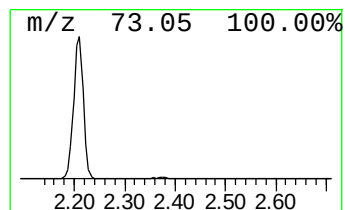
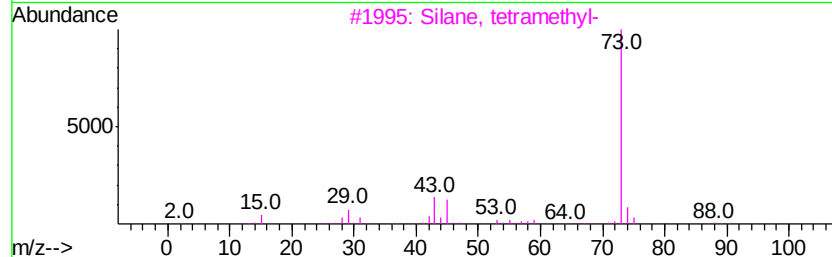
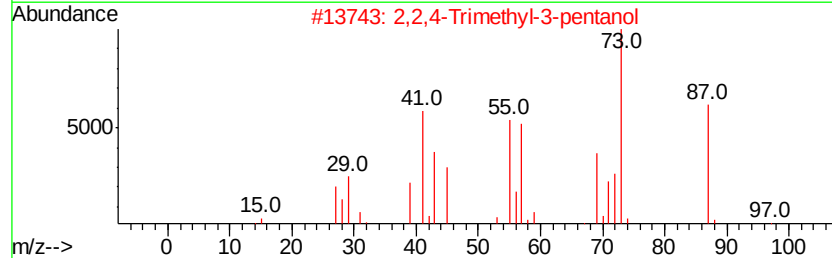
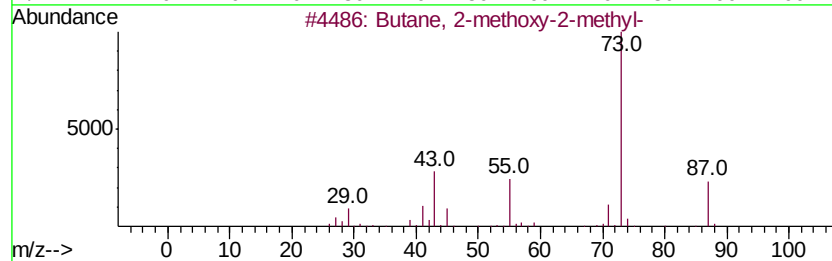
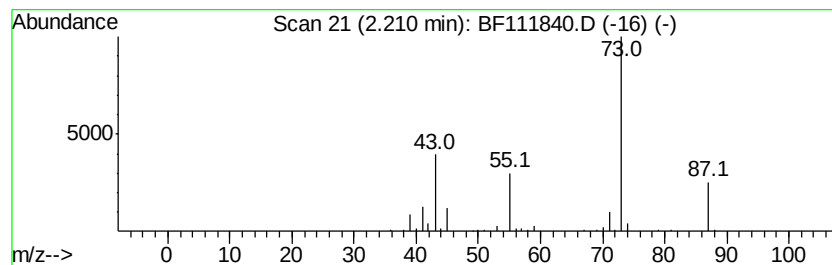
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	2.05 ng	145625	1,4-Dichlorobenzene-d4	6.90

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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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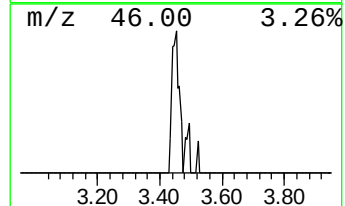
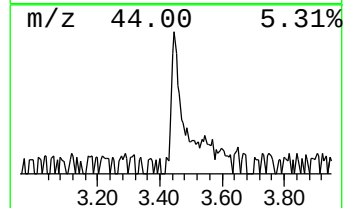
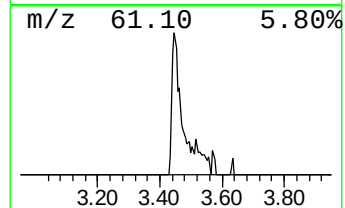
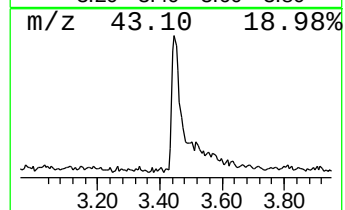
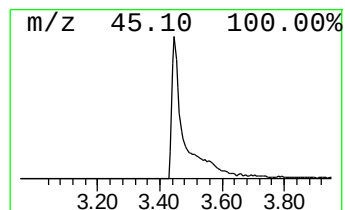
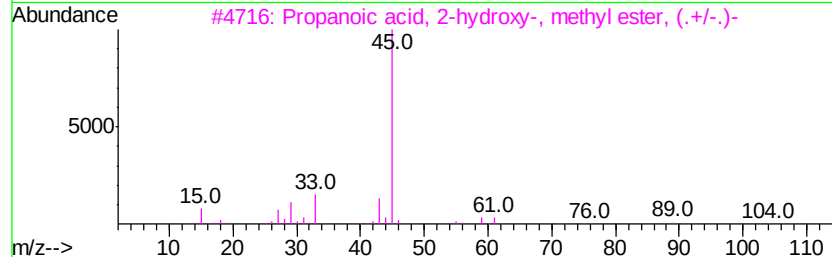
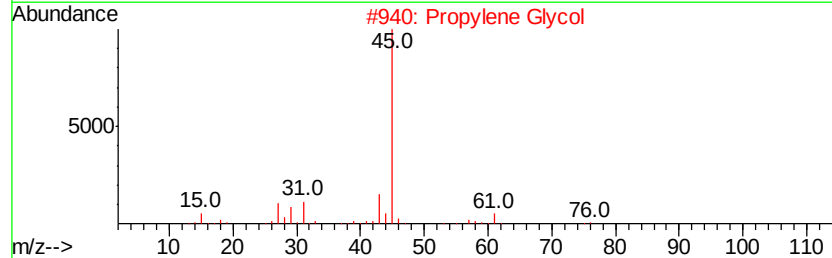
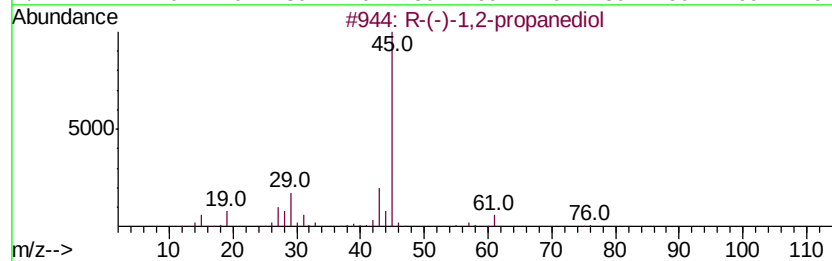
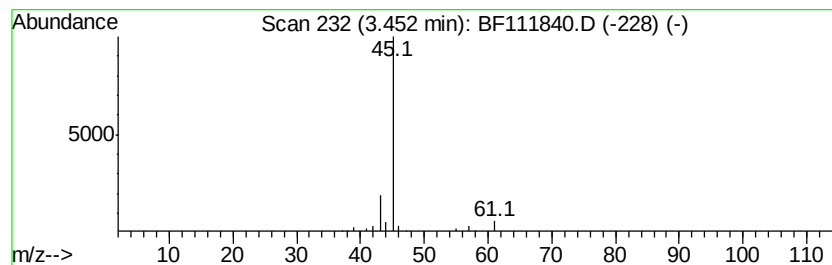
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.45	2.06 ng	146892	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		Propylene Glycol	76	C3H8O2	000057-55-6	9
3		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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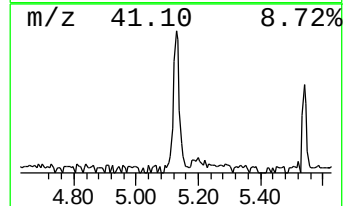
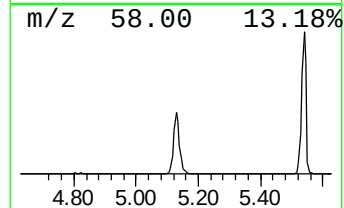
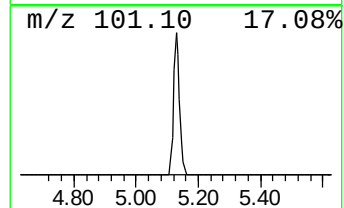
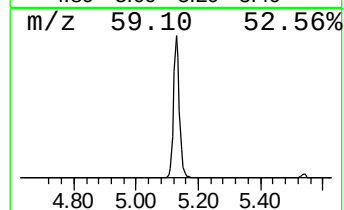
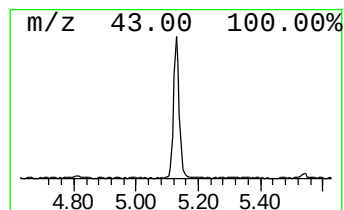
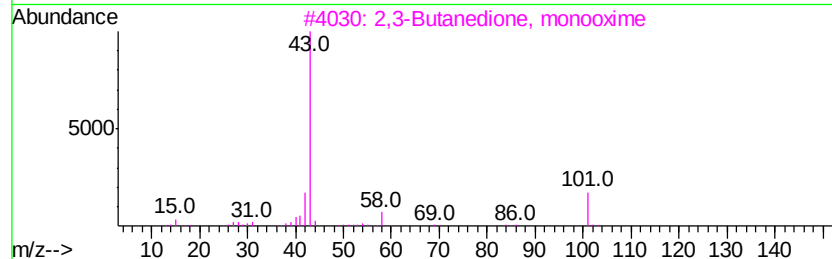
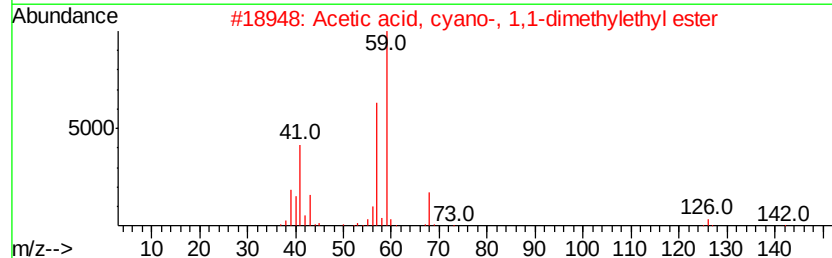
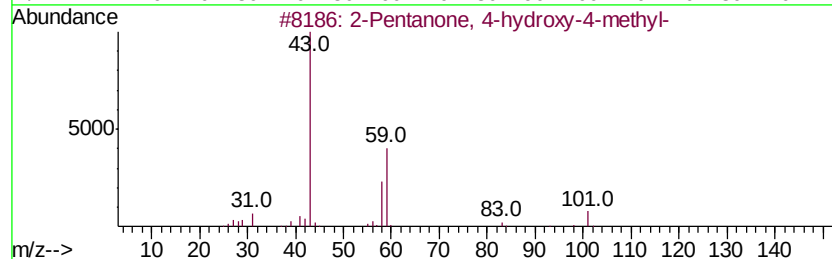
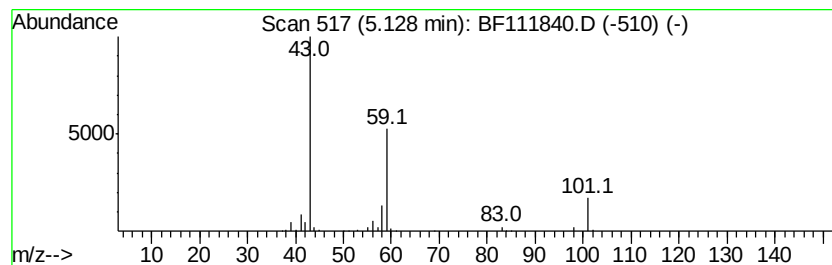
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.50 ng	320459	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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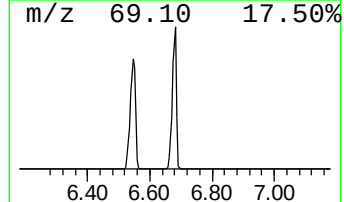
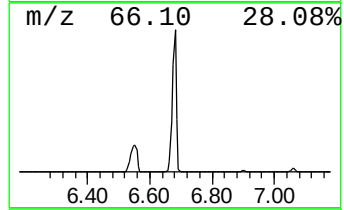
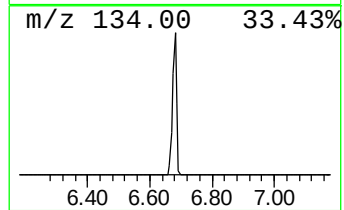
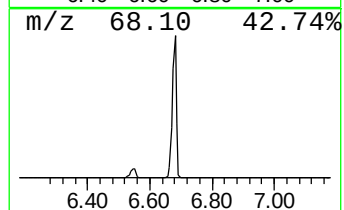
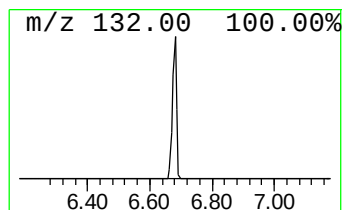
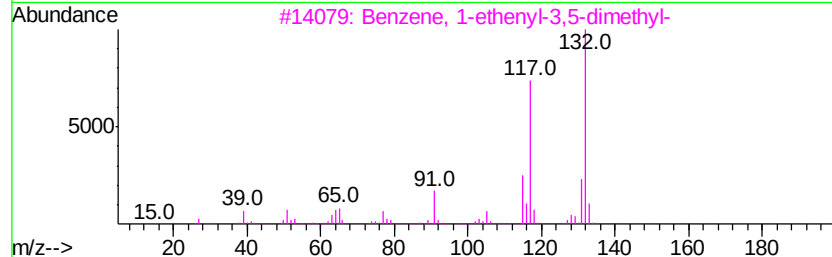
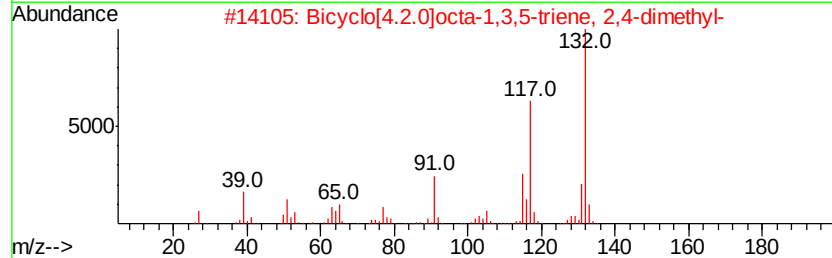
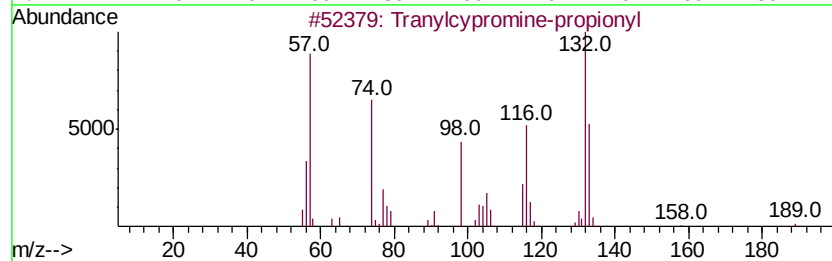
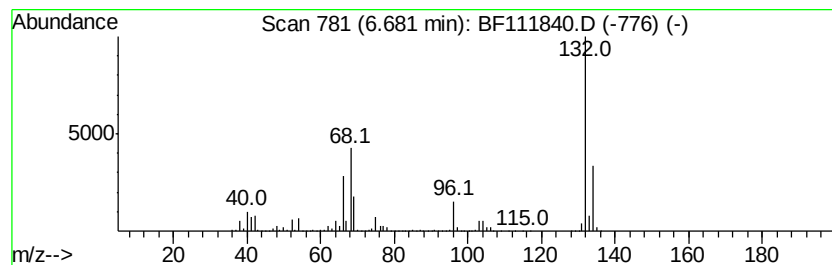
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	74.66 ng	5311720	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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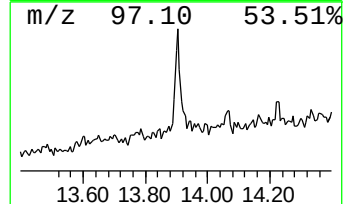
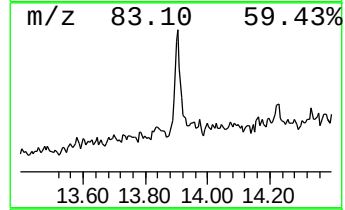
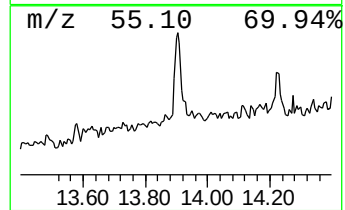
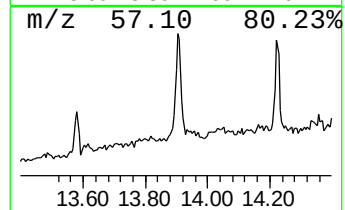
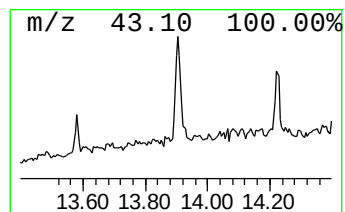
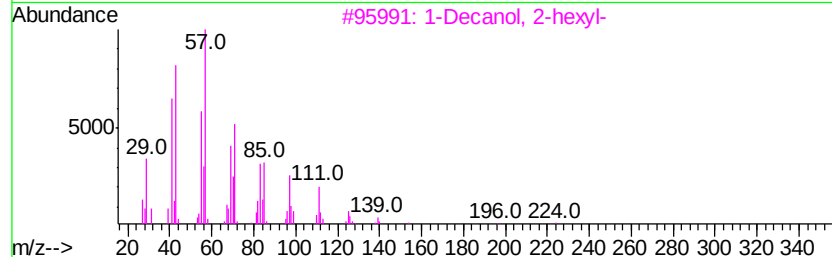
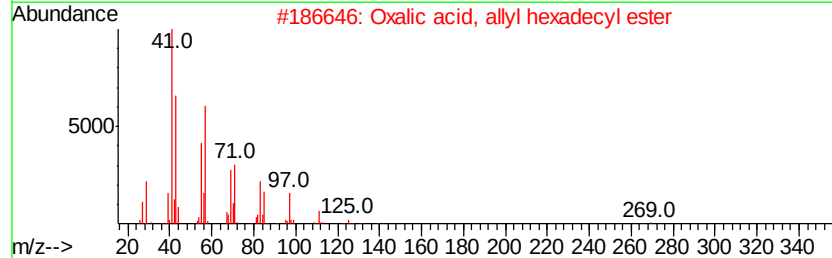
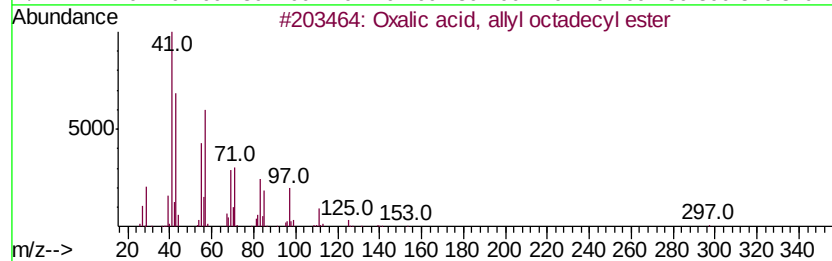
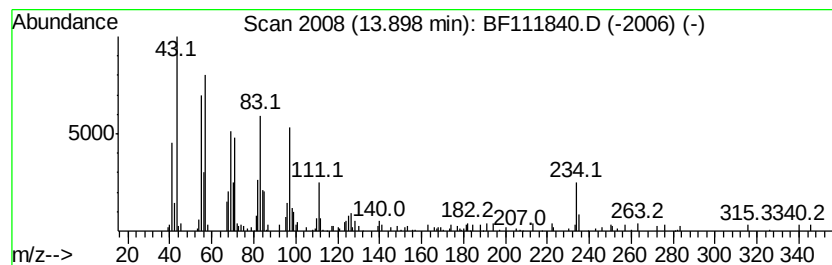
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, allyl octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	2.53 ng	188007	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	83
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	80
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	55
5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	52



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ClientSampleId :
TEST-PIT-D-11-12-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	2.21	2.0	ng	145625	1	6.90	1422980	20.0
R-(-)-1,2-propane...	3.45	2.1	ng	146892	1	6.90	1422980	20.0
2-Pentanone, 4-hy...	5.13	4.5	ng	320459	1	6.90	1422980	20.0
unknown6.68	6.68	74.7	ng	5311720	1	6.90	1422980	20.0
Oxalic acid, ally...	13.90	2.5	ng	188007	5	14.07	1484780	20.0