

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124193.D
 Acq On : 8 Jun 2021 22:23
 Operator : JU/CG
 Sample : M2598-10
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 17

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	314487	334588	63.48%	6.566%
2	2.946	140	146	152	rBV2	51419	78872	14.96%	1.548%
3	3.393	216	222	228	rBV2	38509	81975	15.55%	1.609%
4	4.828	463	466	470	rBB	17682	18494	3.51%	0.363%
5	5.493	575	579	589	rVB	513482	472245	89.60%	9.267%
6	6.504	747	751	760	rBV	490493	450358	85.45%	8.838%
7	6.863	808	812	815	rBV	295577	242647	46.04%	4.762%
8	7.422	903	907	910	rBV	409164	312172	59.23%	6.126%
9	8.145	1026	1030	1033	rBV	344210	270137	51.25%	5.301%
10	9.216	1209	1212	1215	rBV	677120	527052	100.00%	10.343%
11	9.898	1325	1328	1332	rBV	352359	276128	52.39%	5.419%
12	10.328	1398	1401	1405	rVB2	6769	6880	1.31%	0.135%
13	10.686	1459	1462	1468	rVB	327555	273838	51.96%	5.374%
14	10.798	1479	1481	1487	rBV2	7528	9566	1.82%	0.188%
15	11.251	1555	1558	1560	rBV2	8950	7937	1.51%	0.156%
16	11.280	1560	1563	1567	rVB3	5077	7097	1.35%	0.139%
17	11.386	1577	1581	1584	rBV	296181	242108	45.94%	4.751%
18	11.410	1584	1585	1589	rVB	29122	16970	3.22%	0.333%
19	11.622	1617	1621	1624	rBV4	5979	8317	1.58%	0.163%
20	11.674	1627	1630	1634	rBV2	7438	6836	1.30%	0.134%
21	11.922	1668	1672	1677	rVB7	11954	14778	2.80%	0.290%
22	12.210	1718	1721	1723	rBV3	7236	7685	1.46%	0.151%
23	12.392	1749	1752	1756	rBV6	8091	8179	1.55%	0.161%
24	12.469	1764	1765	1770	rBV4	6128	8063	1.53%	0.158%
25	12.527	1772	1775	1781	rBV6	6306	8804	1.67%	0.173%
26	12.604	1784	1788	1792	rBV	47902	46773	8.87%	0.918%
27	12.757	1811	1814	1816	rBV4	7435	7073	1.34%	0.139%
28	12.780	1816	1818	1821	rVB4	8838	8870	1.68%	0.174%
29	12.827	1821	1826	1831	rBV	43272	54953	10.43%	1.078%
30	12.974	1845	1851	1854	rBV	482689	445792	84.58%	8.748%
31	13.051	1860	1864	1867	rVB6	6384	9802	1.86%	0.192%
32	13.133	1876	1878	1880	rBV3	8990	6776	1.29%	0.133%
33	13.204	1887	1890	1891	rBV2	12061	11392	2.16%	0.224%
34	13.263	1897	1900	1903	rBV5	12525	13300	2.52%	0.261%
35	13.351	1914	1915	1920	rBV5	8762	8813	1.67%	0.173%
36	13.416	1924	1926	1930	rBV4	9691	14792	2.81%	0.290%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.457	1930	1933	1937	rBV5	14888	23211	4.40%	0.455%
38	13.551	1944	1949	1950	rBV5	14258	22445	4.26%	0.440%
39	13.657	1965	1967	1974	rVB8	15224	26966	5.12%	0.529%
40	13.827	1994	1996	1998	rBV3	15783	13055	2.48%	0.256%
41	14.033	2024	2031	2034	rBV	283611	297145	56.38%	5.831%
42	14.057	2034	2035	2038	rVB2	31731	18062	3.43%	0.354%
43	15.080	2207	2209	2211	rBV3	24623	22599	4.29%	0.443%
44	15.515	2279	2283	2291	rVB3	169139	238988	45.34%	4.690%
45	15.974	2359	2361	2366	rVB5	26589	29979	5.69%	0.588%
46	16.321	2418	2420	2421	rVB2	17030	9940	1.89%	0.195%
47	17.086	2548	2550	2551	rBV2	19681	16505	3.13%	0.324%
48	17.521	2622	2624	2625	rBV2	15412	13842	2.63%	0.272%
49	17.709	2655	2656	2658	rBV2	14670	8545	1.62%	0.168%
50	17.733	2658	2660	2662	rBV3	10125	6508	1.23%	0.128%
51	17.945	2694	2696	2698	rVB3	15006	10899	2.07%	0.214%
52	18.209	2739	2741	2744	rBV4	11284	10462	1.99%	0.205%
53	18.692	2821	2823	2824	rBV2	9460	6612	1.25%	0.130%

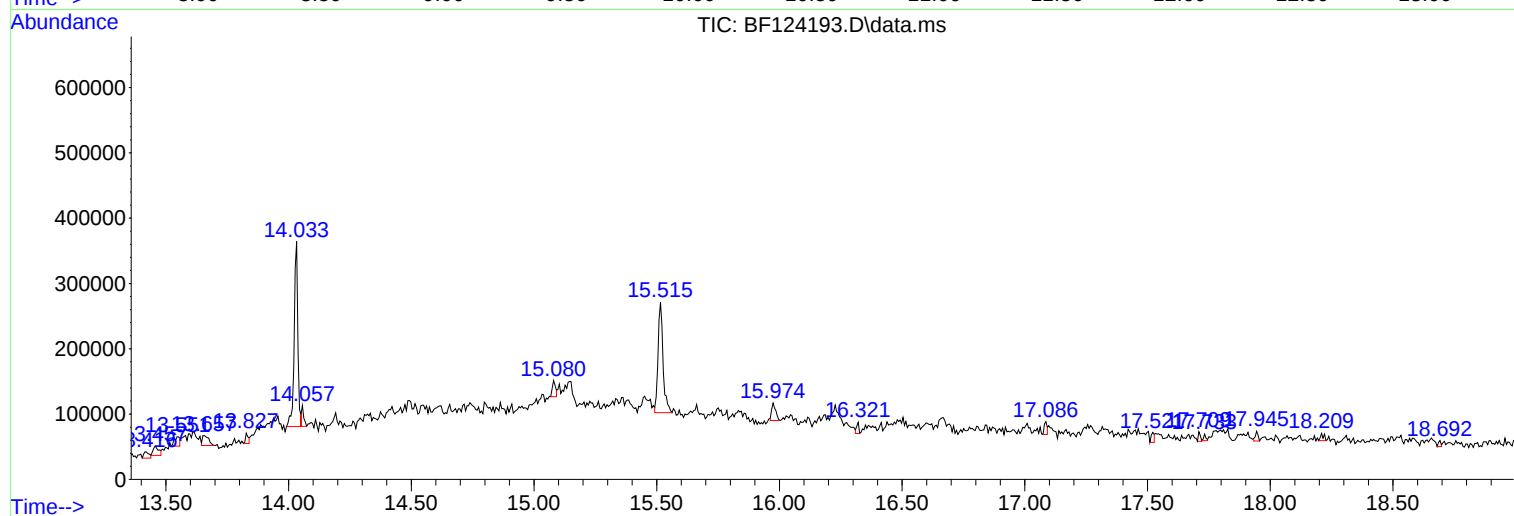
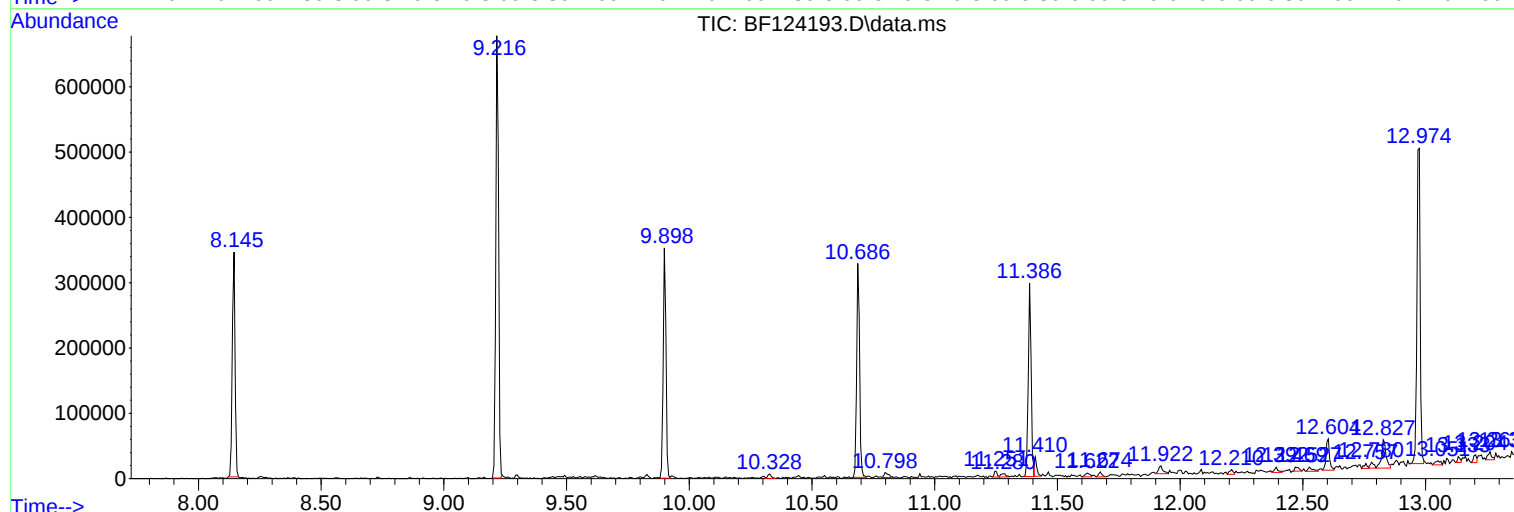
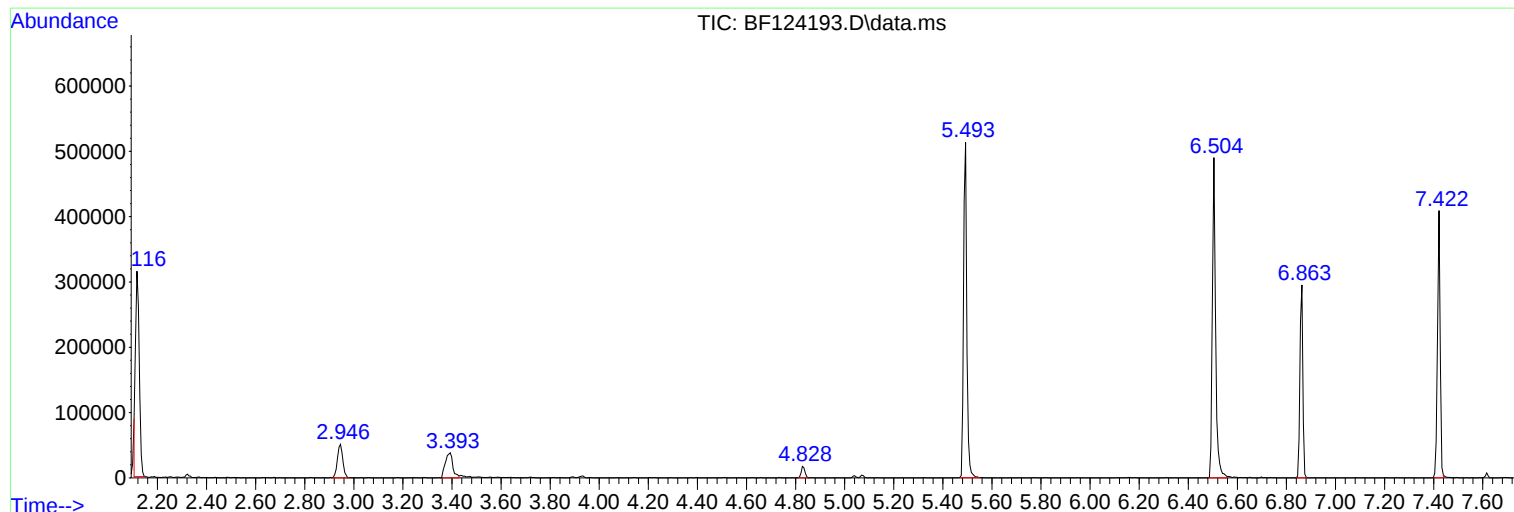
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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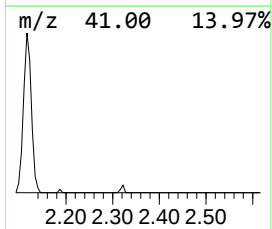
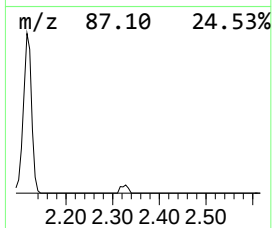
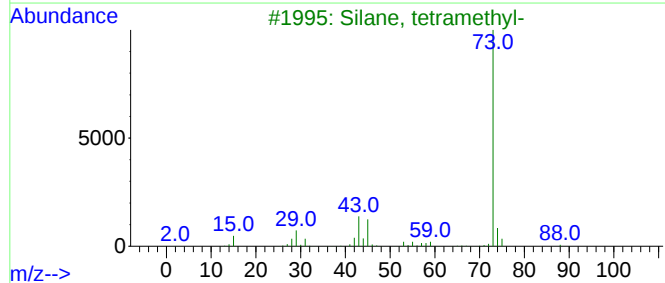
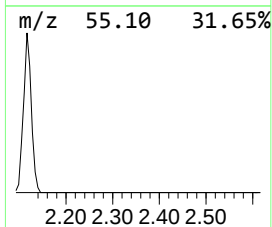
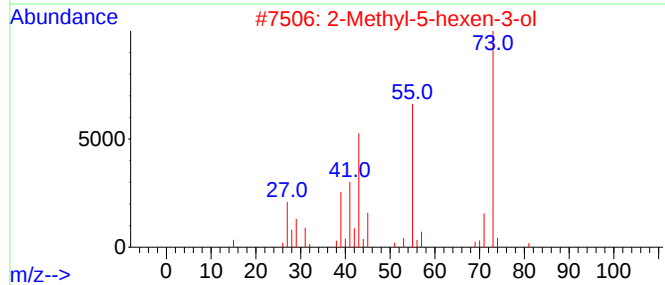
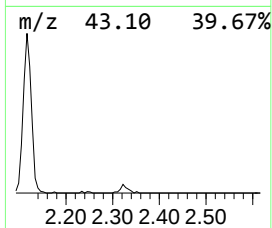
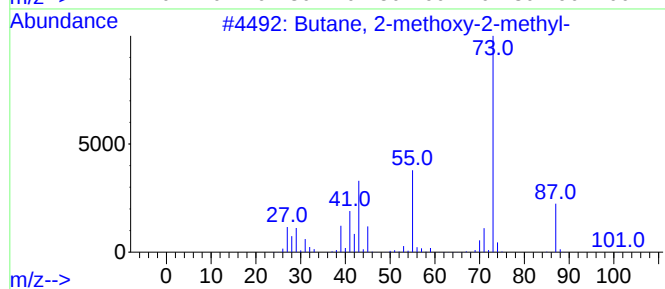
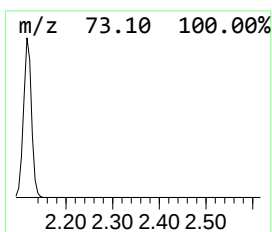
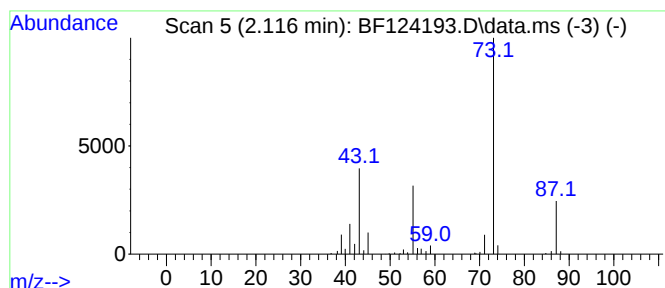
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	27.58 ng	334588	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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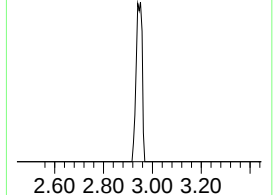
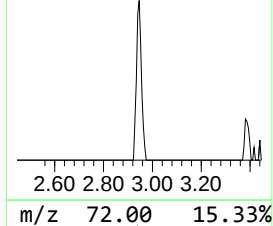
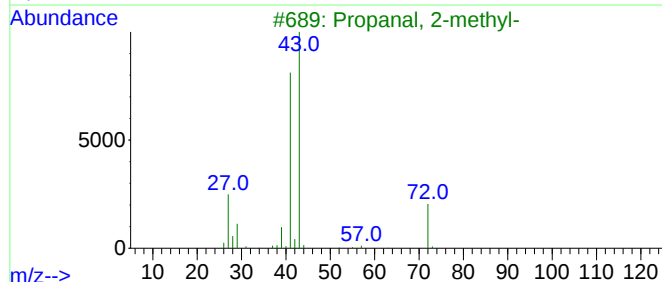
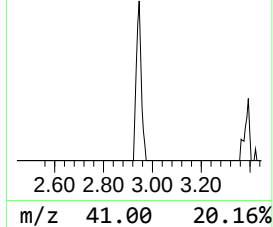
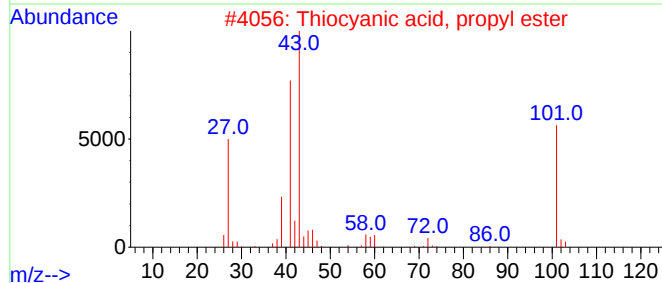
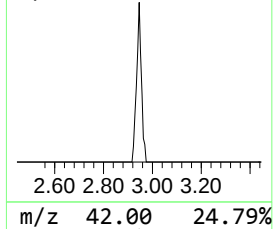
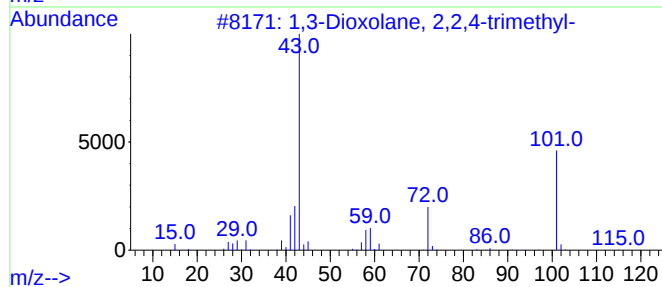
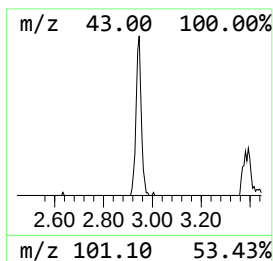
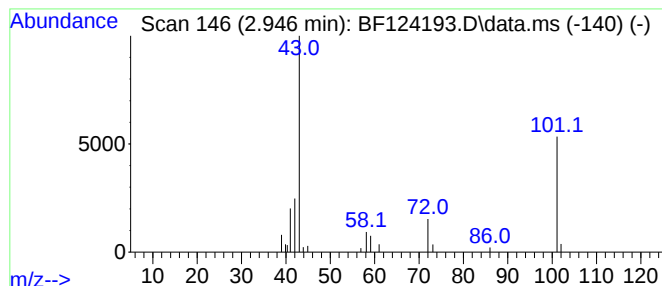
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.946	6.50 ng	78872	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	72
2		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	42
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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ALS Vial : 11 Sample Multiplier: 1

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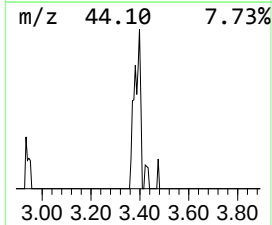
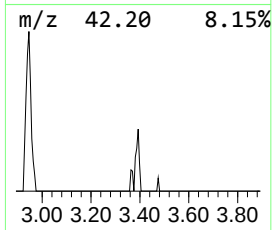
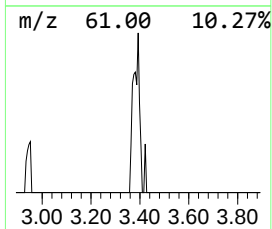
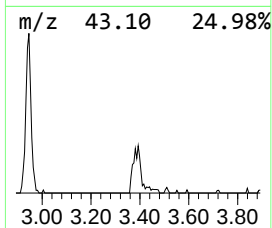
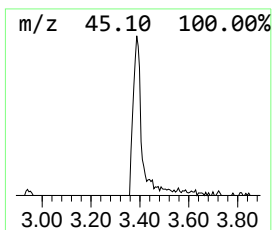
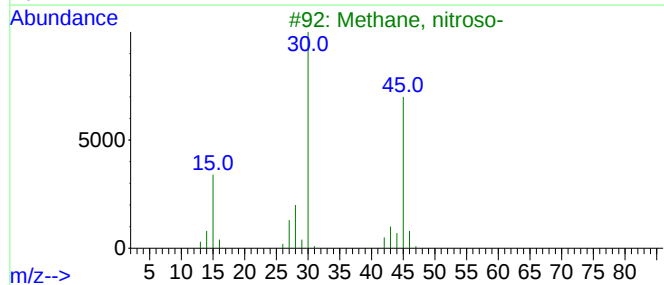
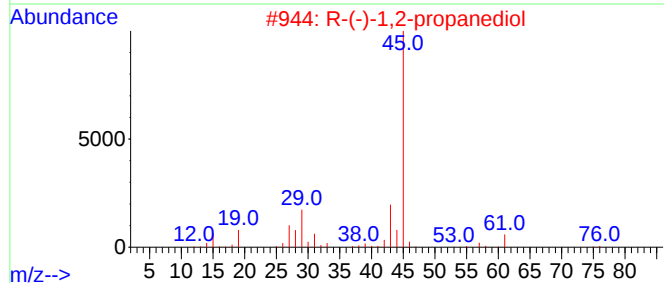
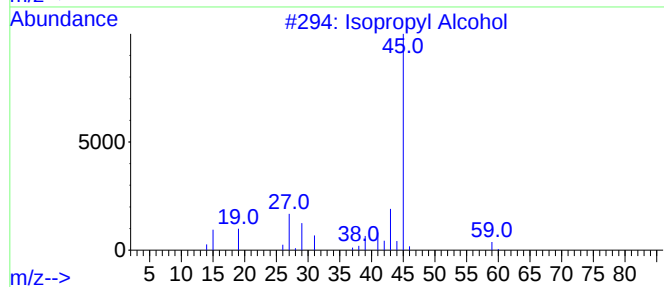
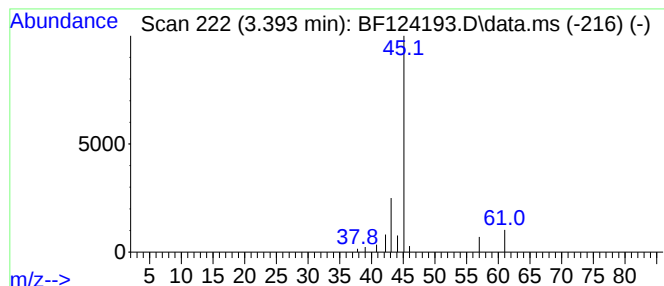
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown3.393 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	6.76 ng	81975	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Propylene Glycol	76	C3H8O2	000057-55-6	4
5			2-Butanol	74	C4H10O	000078-92-2	4



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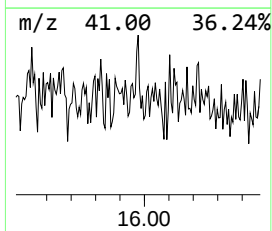
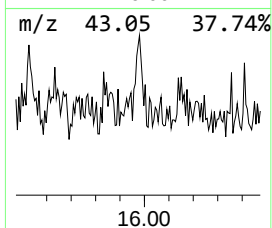
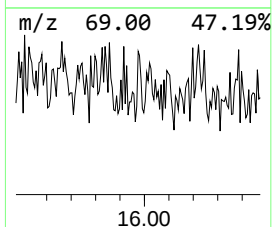
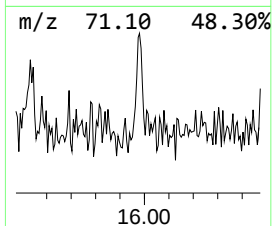
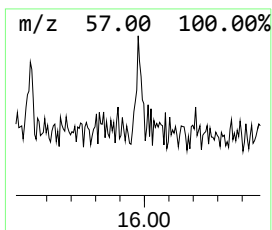
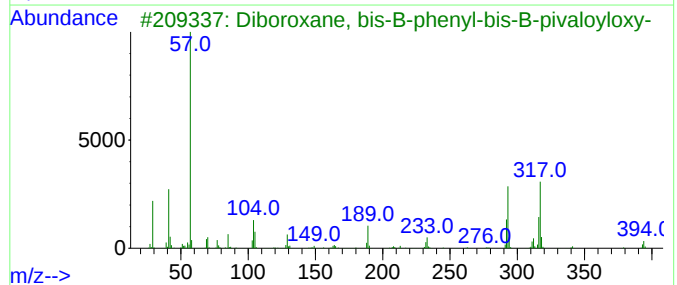
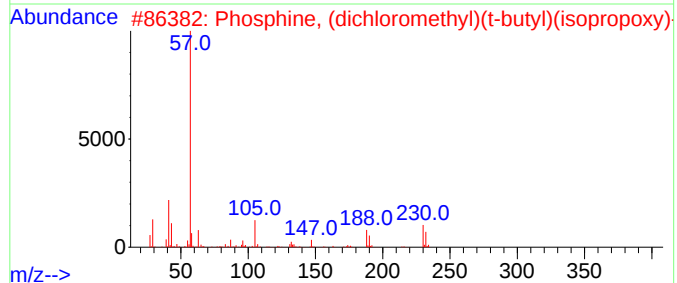
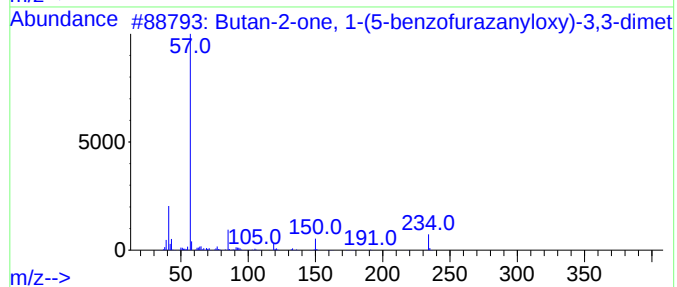
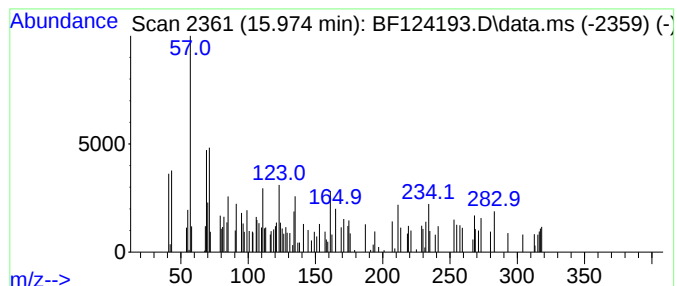
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.974 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.51 ng	29979	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butan-2-one, 1-(5-benzofurazanyl...	234	C12H14N2O3	329933-46-2	9		
2	Phosphine, (dichloromethyl)(t-bu...	230	C8H17Cl2OP	1000162-70-0	9		
3	Diboroxane, bis-B-phenyl-bis-B-p...	394	C22H28B2O5	1000151-19-3	2		
4	1-Methoxy-3,4-dimethyl-1-phenyl-...	264	C13H18GeO	026311-84-2	2		
5	Phosphine sulfide, (chloro)(t-bu...	232	C10H14ClPS	115591-17-8	2		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.116	27.6	ng	334588	1	6.863	242647	20.0
1,3-Dioxolane, ...	2.946	6.5	ng	78872	1	6.863	242647	20.0
unknown3.393	3.393	6.8	ng	81975	1	6.863	242647	20.0
unknown15.974	15.974	2.5	ng	29979	6	15.515	238988	20.0