

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033023\
 Data File : BM039223.D
 Acq On : 30 Mar 2023 12:34
 Operator : CG/JU
 Sample : 01950-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PT-ACIDS-WP

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_M\Methods\8270-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.887	98	102	110	rVB	110635	131692	1.01%	0.083%
2	5.016	287	294	301	rBV	2382774	3309586	25.50%	2.097%
3	5.481	367	373	390	rBV	5535532	7845371	60.45%	4.971%
4	7.098	640	648	650	rBV	4728256	8826359	68.01%	5.593%
5	7.122	650	652	667	rVB	6196158	7720810	59.49%	4.892%
6	7.487	707	714	734	rVB	4464306	6892330	53.11%	4.367%
7	7.922	781	788	799	rBV	849403	1308354	10.08%	0.829%
8	8.375	857	865	884	rBV	3958909	6166740	47.52%	3.907%
9	9.092	979	987	994	rBV	3138956	5070177	39.07%	3.213%
10	9.851	1108	1116	1121	rBV	3359242	5425457	41.81%	3.438%
11	9.910	1121	1126	1141	rVB	1849334	2949494	22.73%	1.869%
12	10.381	1199	1206	1228	rBV	4258113	7150404	55.10%	4.531%
13	10.733	1259	1266	1277	rVB	1062245	1717976	13.24%	1.089%
14	10.916	1289	1297	1313	rBV	3562399	5843341	45.03%	3.703%
15	12.022	1476	1485	1500	rBV	3092674	4890061	37.68%	3.098%
16	13.004	1645	1652	1659	rBV	5567611	8347113	64.32%	5.289%
17	13.074	1659	1664	1677	rVV	1917065	3076760	23.71%	1.950%
18	13.198	1677	1685	1695	rVB	6940221	10368694	79.90%	6.570%
19	14.568	1911	1918	1929	rBV	1355711	1997919	15.40%	1.266%
20	14.686	1932	1938	1949	rBV	2603351	3804613	29.32%	2.411%
21	14.792	1949	1956	1985	rVB	3629234	5717110	44.05%	3.623%
22	15.198	2018	2025	2044	rBV	4713928	6637550	51.15%	4.206%
23	15.698	2104	2110	2123	rBV	3653990	5192183	40.01%	3.290%
24	16.062	2165	2172	2191	rBV	5260028	7367081	56.77%	4.668%
25	16.968	2319	2326	2348	rBV	7137510	10049320	77.44%	6.368%
26	17.315	2379	2385	2397	rBV	1522326	2178507	16.79%	1.380%
27	19.945	2826	2832	2850	rBV	10594842	12977257	100.00%	8.223%
28	21.503	3092	3097	3106	rBV	1741007	2277710	17.55%	1.443%
29	23.915	3501	3507	3522	rVB2	1222966	2580748	19.89%	1.635%

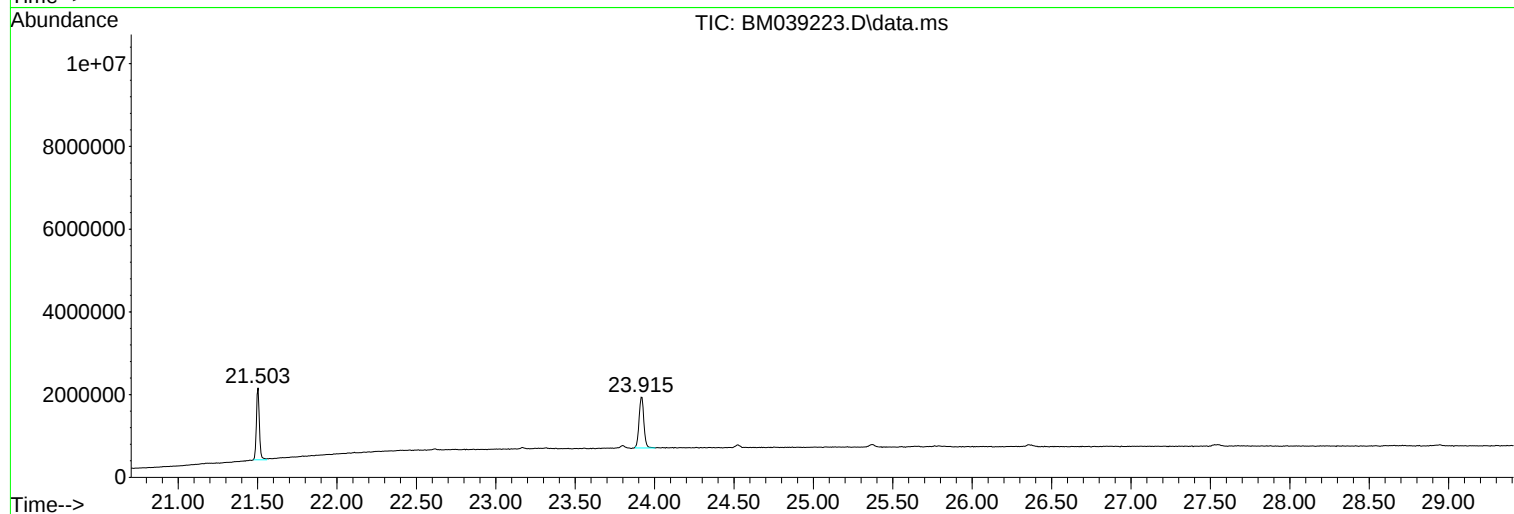
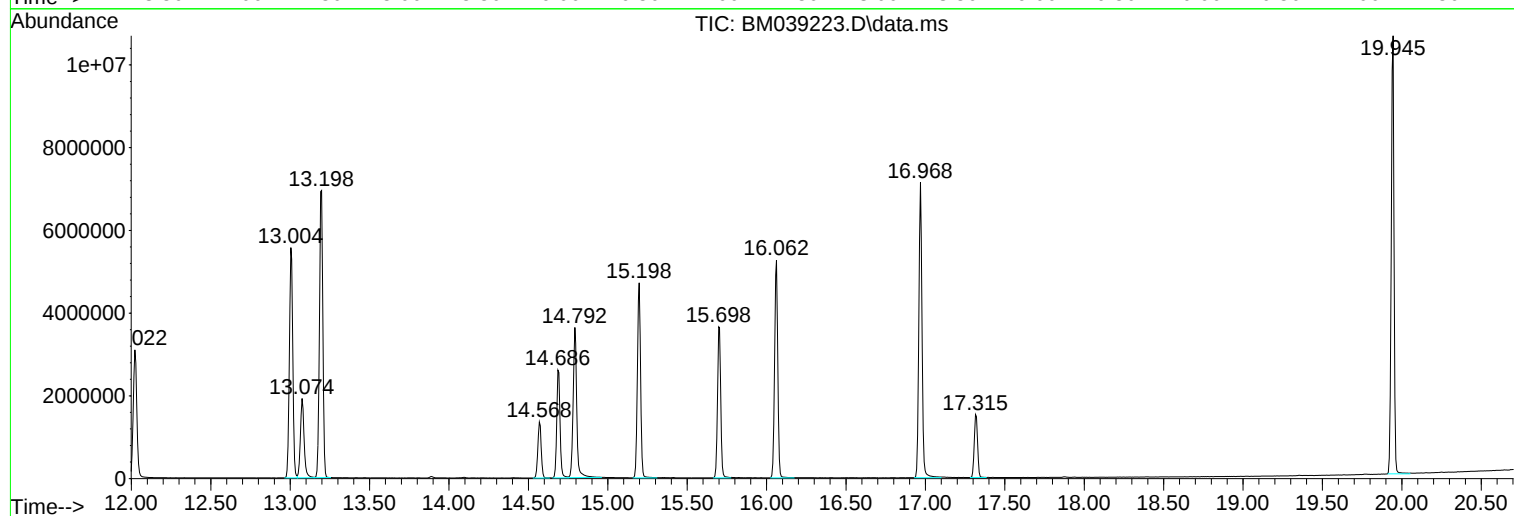
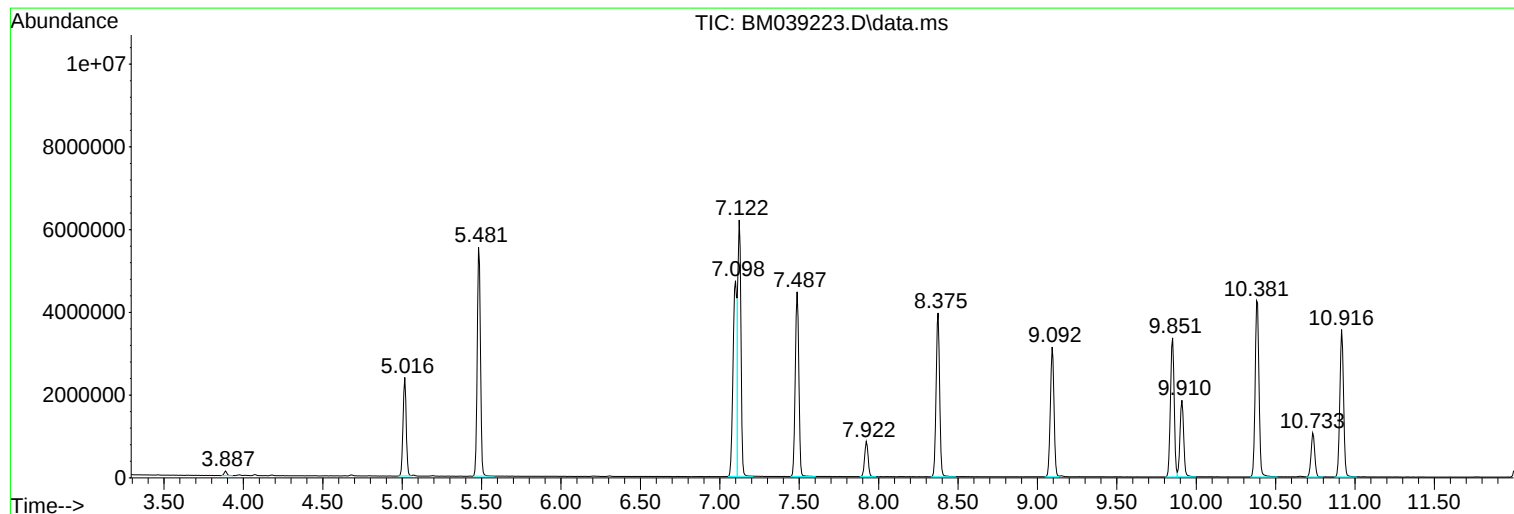
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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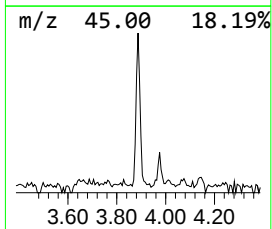
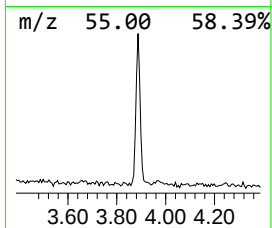
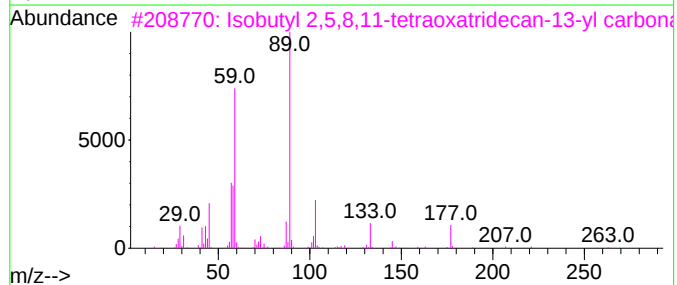
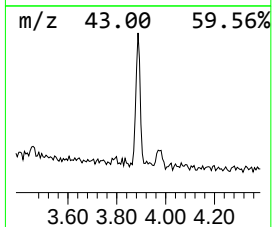
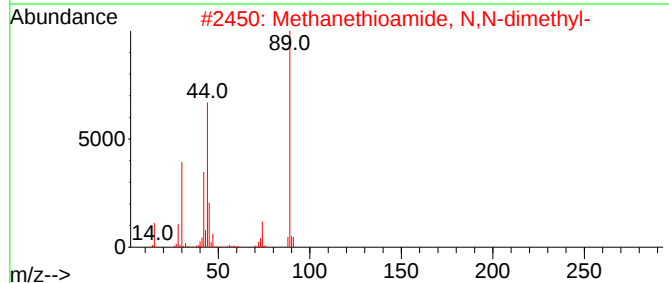
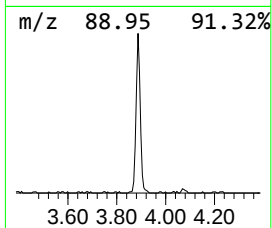
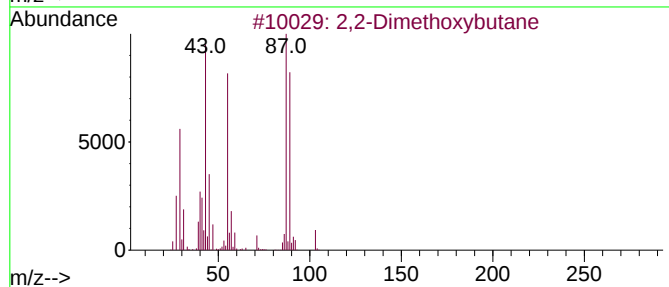
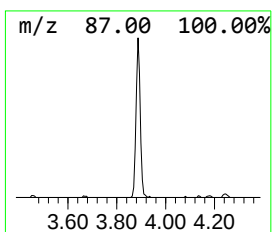
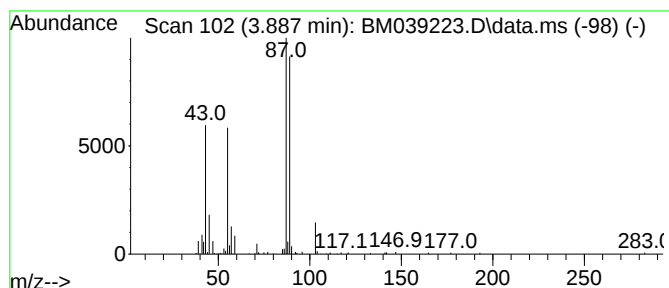
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,2-Dimethoxybutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.887	2.01 ng	131692	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethoxybutane	118	C6H14O2	003453-99-4	74
2			Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	59
3			Isobutyl 2,5,8,11-tetraoxatridec...	308	C14H28O7	1000378-27-9	45
4			2,2-Dimethoxypropionamide	133	C5H11NO3	1000237-69-7	38
5			Isobutyl (2-(2-methoxyethoxy)...	264	C12H24O6	1000378-28-5	38



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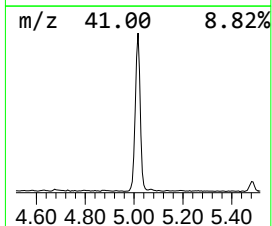
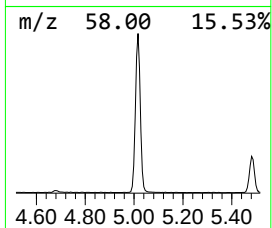
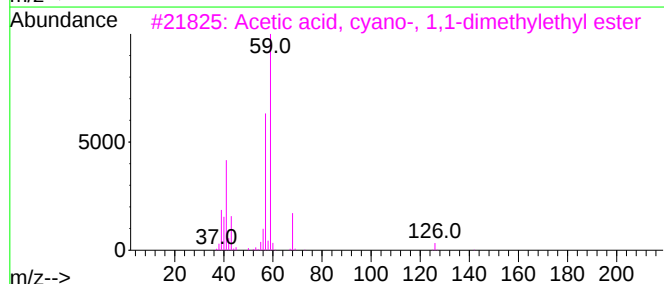
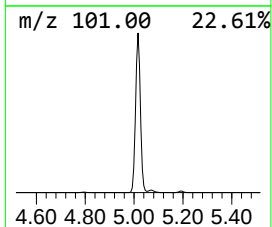
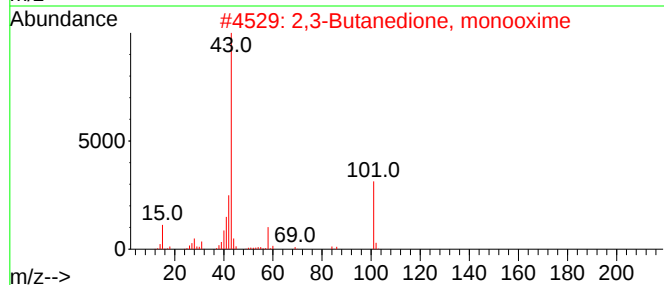
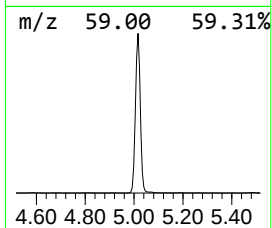
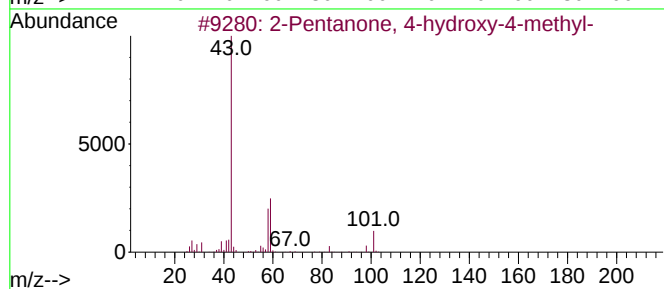
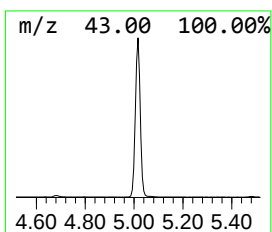
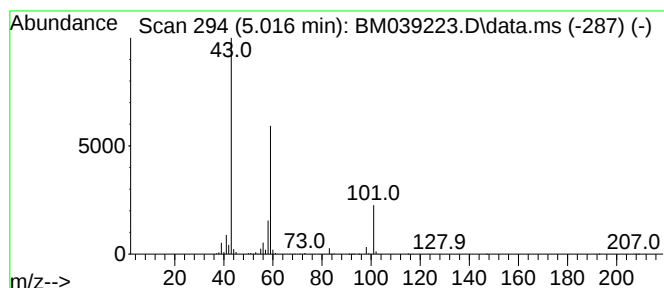
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	50.59 ng	3309590	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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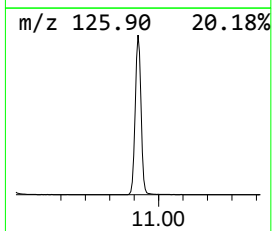
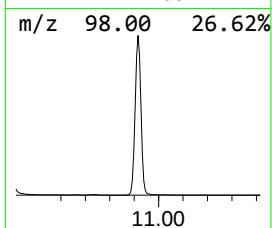
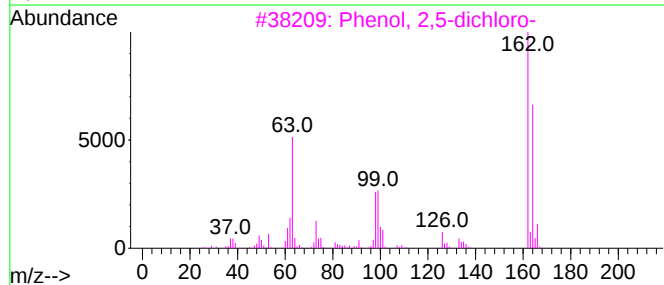
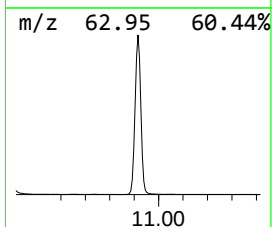
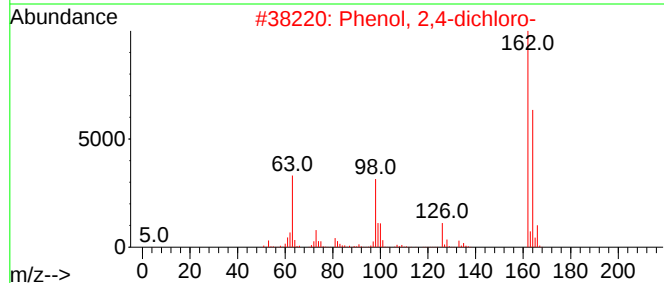
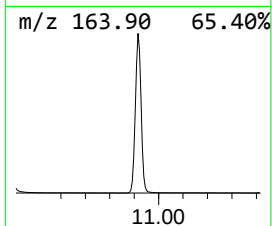
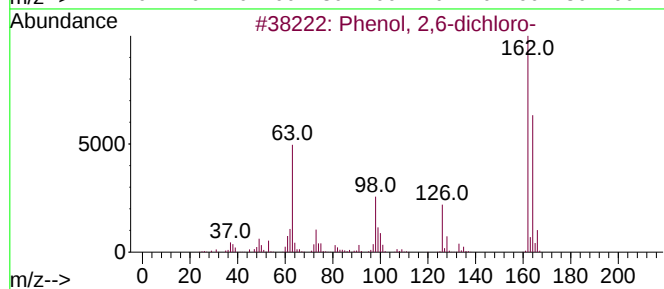
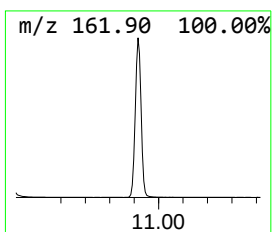
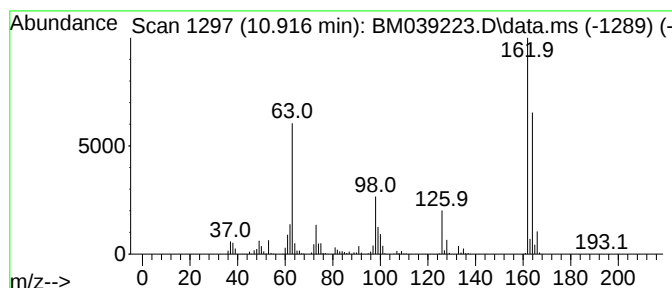
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenol, 2,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.916	68.03 ng	5843340	Naphthalene-d8	10.733	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	98
2	Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	97
3	Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	94
4	Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	91
5	Phenol, 3,5-dichloro-	162	C6H4Cl2O	000591-35-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,2-Dimethoxybu...	3.887	2.0	ng	131692	1	7.922	1308350	20.0
2-Pentanone, 4-...	5.016	50.6	ng	3309590	1	7.922	1308350	20.0
Phenol, 2,6-dic...	10.916	68.0	ng	5843340	2	10.733	1717980	20.0