

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012323\
 Data File : BG056394.D
 Acq On : 23 Jan 2023 21:52
 Operator : CG/JU
 Sample : 01253-01 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-04-012023

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_G\Methods\8270-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.332	341	348	357	rBV	53836	87128	7.08%	0.983%
2	5.820	424	431	441	rBV	244191	409943	33.30%	4.627%
3	7.436	699	706	720	rBV	244732	439717	35.72%	4.963%
4	8.299	846	853	862	rVB	158475	271225	22.03%	3.062%
5	9.469	1045	1052	1062	rBV	149550	265681	21.58%	2.999%
6	11.131	1326	1335	1342	rBV	214415	400888	32.56%	4.525%
7	11.249	1350	1355	1363	rVB4	7943	14018	1.14%	0.158%
8	11.807	1442	1450	1454	rBV7	7223	14119	1.15%	0.159%
9	12.107	1495	1501	1506	rBV2	12758	20948	1.70%	0.236%
10	13.117	1668	1673	1678	rBV8	6790	15808	1.28%	0.178%
11	13.423	1721	1725	1730	rBV3	24909	41583	3.38%	0.469%
12	13.534	1737	1744	1755	rVB	570537	880724	71.54%	9.942%
13	13.705	1769	1773	1775	rBV4	8491	13549	1.10%	0.153%
14	13.946	1810	1814	1818	rBV7	10351	15178	1.23%	0.171%
15	14.075	1830	1836	1837	rBV5	16467	24548	1.99%	0.277%
16	14.234	1858	1863	1867	rVV2	32380	57923	4.70%	0.654%
17	14.281	1867	1871	1875	rVV3	21108	35619	2.89%	0.402%
18	14.333	1875	1880	1882	rVV2	25926	38759	3.15%	0.438%
19	14.357	1882	1884	1890	rVB3	28226	36503	2.97%	0.412%
20	14.463	1898	1902	1908	rBV6	12120	21526	1.75%	0.243%
21	14.645	1927	1933	1938	rBV8	15516	30142	2.45%	0.340%
22	14.739	1945	1949	1953	rVB3	14843	22741	1.85%	0.257%
23	14.909	1972	1978	1987	rVB	381699	614442	49.91%	6.936%
24	15.109	2006	2012	2020	rVB2	20191	49358	4.01%	0.557%
25	15.185	2021	2025	2029	rBV7	9728	15482	1.26%	0.175%
26	15.297	2040	2044	2048	rVB	27024	39305	3.19%	0.444%
27	15.373	2051	2057	2061	rBV	29020	46180	3.75%	0.521%
28	15.514	2076	2081	2086	rBV2	30554	53298	4.33%	0.602%
29	15.567	2086	2090	2095	rVB2	20341	28500	2.31%	0.322%
30	15.691	2104	2111	2113	rBV7	19038	36567	2.97%	0.413%
31	15.908	2143	2148	2150	rBV6	6923	12866	1.05%	0.145%
32	15.932	2150	2152	2158	rVV6	10264	22620	1.84%	0.255%
33	15.984	2158	2161	2168	rVB3	11439	25557	2.08%	0.288%
34	16.073	2174	2176	2179	rBV3	11799	16461	1.34%	0.186%
35	16.114	2179	2183	2186	rVV4	24200	34487	2.80%	0.389%
36	16.155	2186	2190	2196	rVB6	12856	19119	1.55%	0.216%

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37	16.249	2202	2206	2212	rVB3	39316	62571	5.08%	0.706%
38	16.390	2225	2230	2237	rBV	328206	511726	41.57%	5.776%
39	16.596	2259	2265	2273	rVB5	44321	83143	6.75%	0.939%
40	16.748	2286	2291	2296	rBV4	15636	26703	2.17%	0.301%
41	17.007	2331	2335	2340	rBV4	18026	35483	2.88%	0.401%
42	17.289	2379	2383	2387	rBV7	11959	20407	1.66%	0.230%
43	17.412	2400	2404	2408	rVB	19865	28813	2.34%	0.325%
44	17.647	2438	2444	2449	rBV	486006	728883	59.20%	8.228%
45	17.688	2449	2451	2456	rVB2	24473	34223	2.78%	0.386%
46	17.841	2474	2477	2481	rVB6	11802	15608	1.27%	0.176%
47	18.493	2584	2588	2596	rBV5	63312	138796	11.27%	1.567%
48	18.564	2597	2600	2608	rVB	31669	47725	3.88%	0.539%
49	18.699	2620	2623	2628	rBV5	14264	19321	1.57%	0.218%
50	19.416	2741	2745	2748	rBV	29516	41445	3.37%	0.468%
51	19.680	2787	2790	2794	rVB	47347	58852	4.78%	0.664%
52	19.745	2799	2801	2806	rBV6	15385	25274	2.05%	0.285%
53	20.039	2848	2851	2859	rVB2	51619	80377	6.53%	0.907%
54	20.103	2859	2862	2865	rBV2	17801	21601	1.75%	0.244%
55	20.221	2877	2882	2888	rVB	984209	1231122	100.00%	13.897%
56	21.936	3168	3174	3180	rBV2	442571	760997	61.81%	8.590%
57	25.373	3753	3759	3770	rVB3	250873	713460	57.95%	8.053%

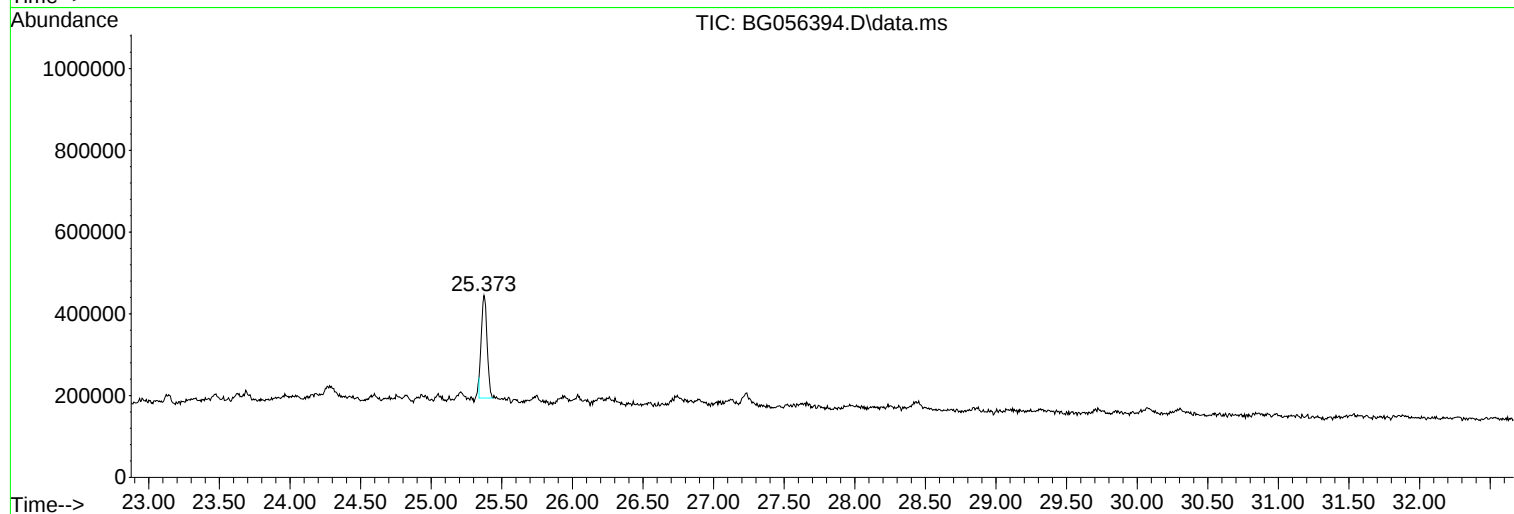
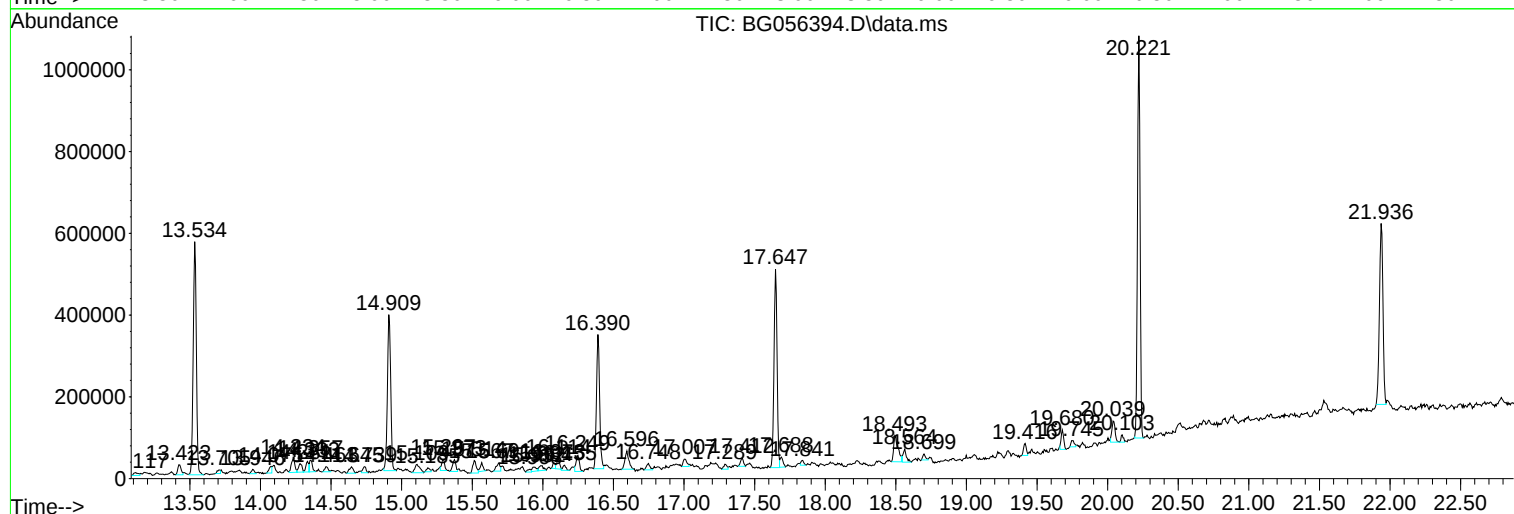
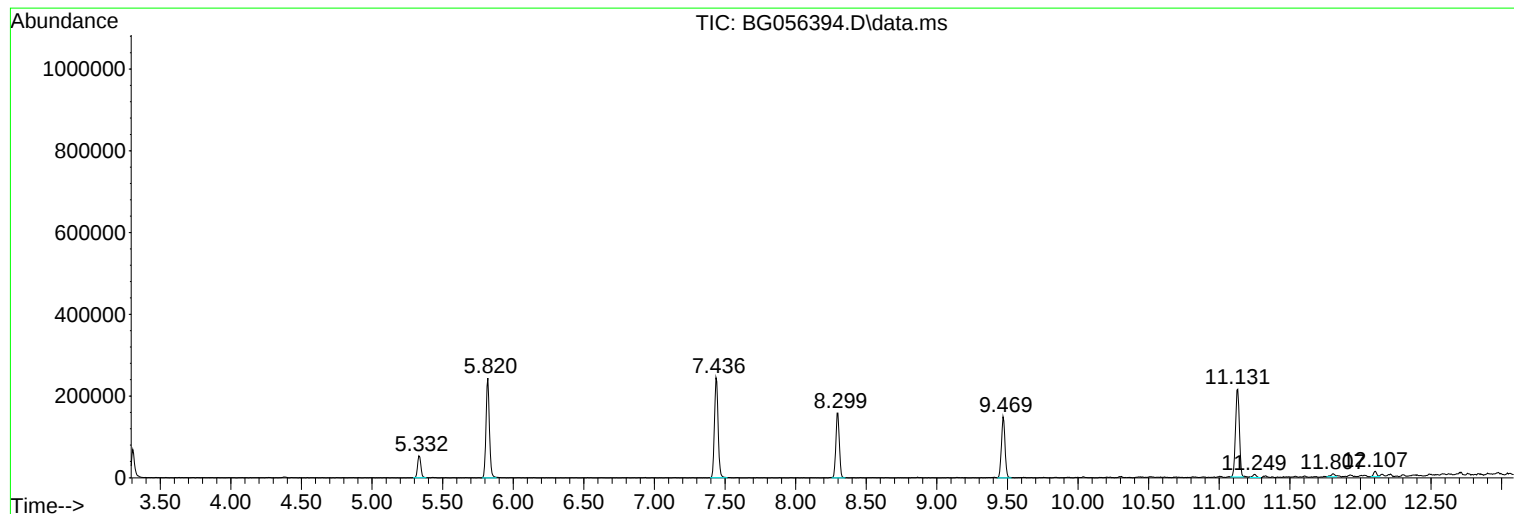
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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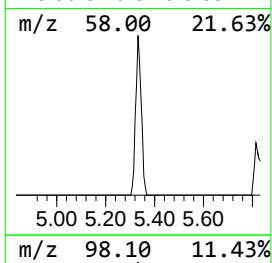
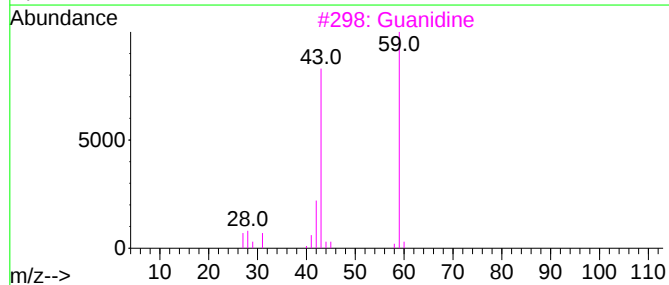
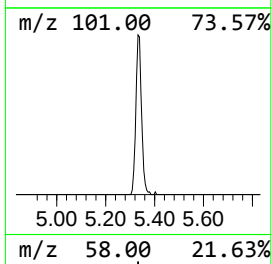
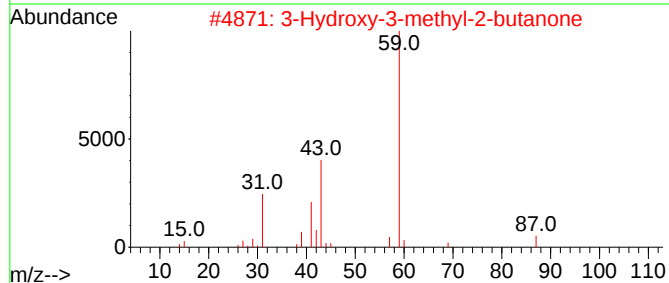
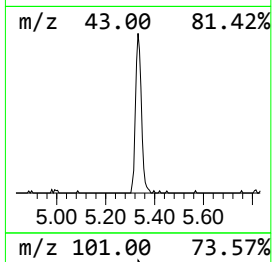
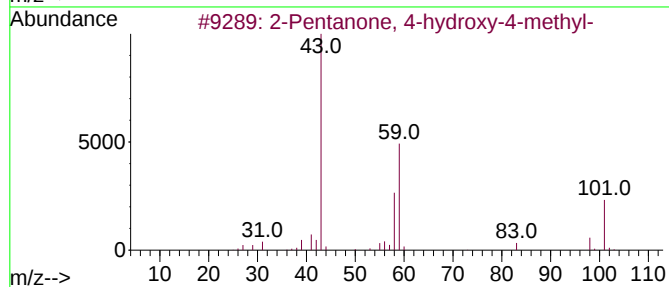
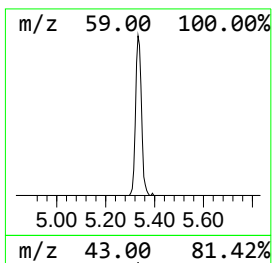
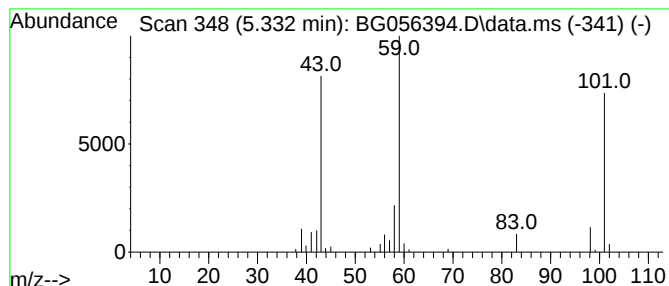
Instrument :
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ClientSampleId :
SU-04-012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.332	6.42 ng	87128	1,4-Dichlorobenzene-d4		8.299	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	3-Hydroxy-3-methyl-2-butanone		102	C5H10O2	000115-22-0	27
3	Guanidine		59	CH5N3	000113-00-8	17
4	Propane, 1-ethoxy-2-methyl-		102	C6H14O	000627-02-1	16
5	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	12



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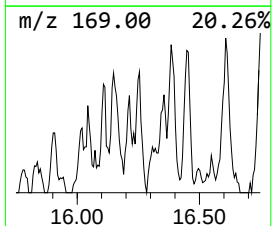
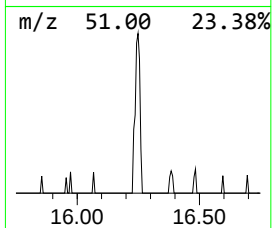
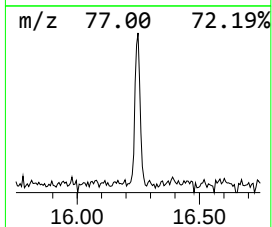
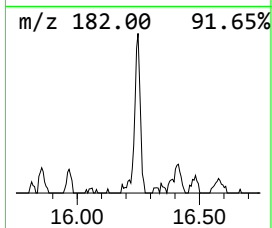
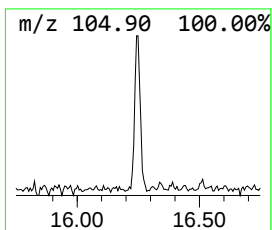
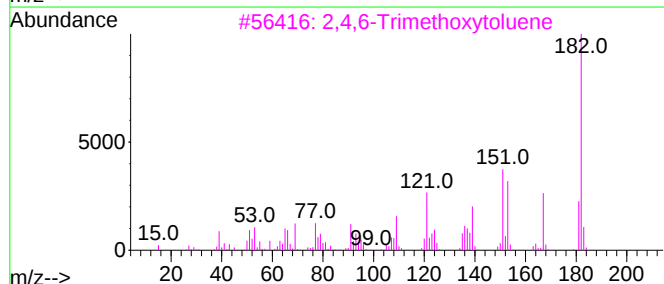
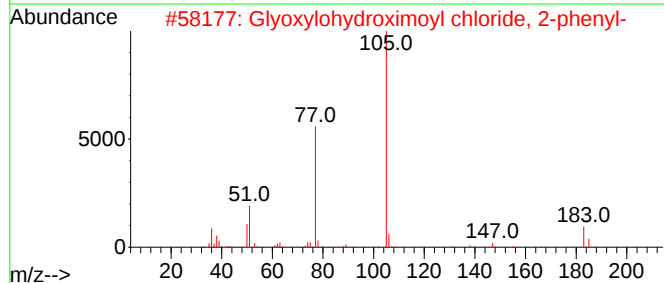
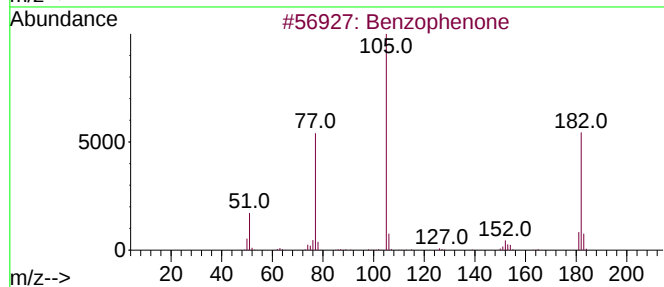
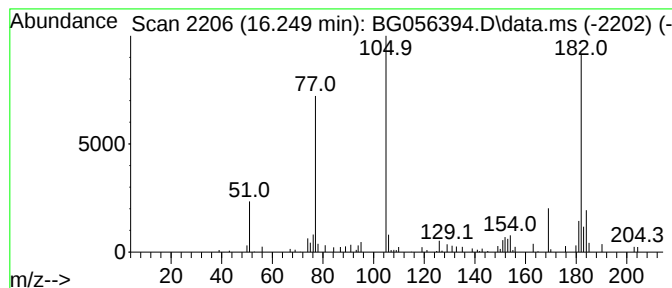
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.249	2.04 ng	62571	Acenaphthene-d10	14.909

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	76
2			Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	30
3			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	30
4			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	27
5			Pyrido[2,3-b]indole, 6-methyl-	182	C12H10N2	108349-67-3	27



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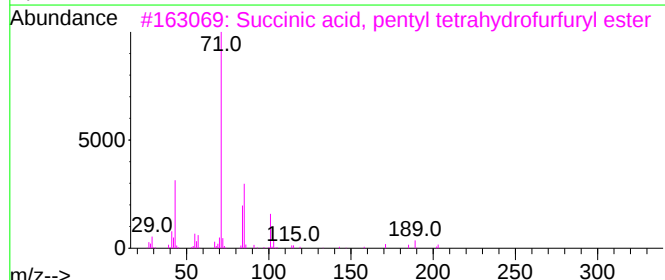
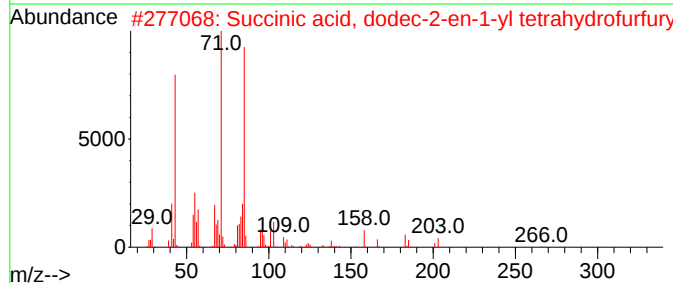
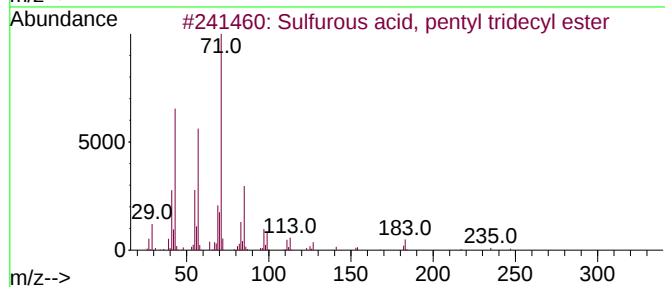
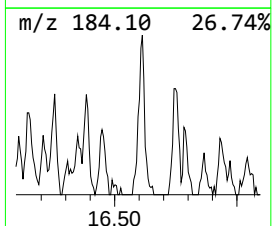
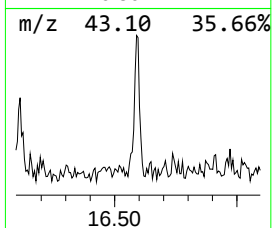
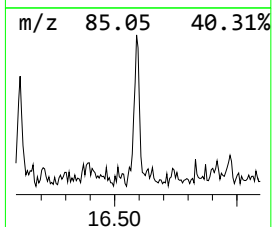
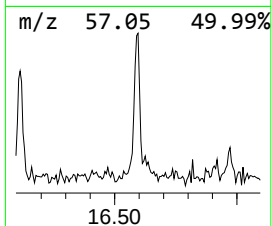
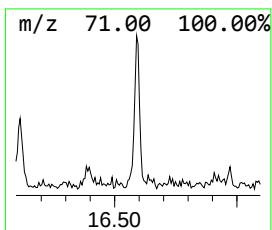
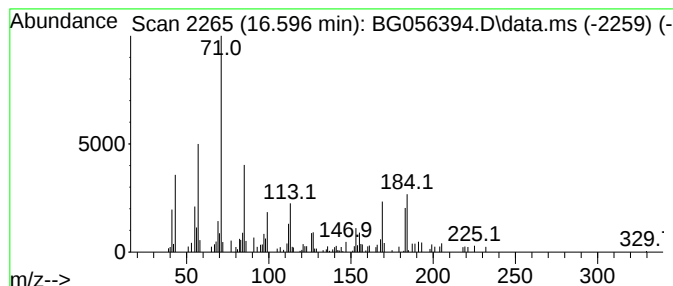
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Sulfurous acid, pentyl trid... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.596	2.28 ng	83143	Phenanthrene-d10	17.647

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, pentyl tridecyl ...	334	C18H38O3S	1000309-14-6	53
2			Succinic acid, dodec-2-en-1-yl t...	368	C21H36O5	1000390-72-8	43
3			Succinic acid, pentyl tetrahydro...	272	C14H24O5	1000329-86-3	38
4			Succinic acid, dodecyl tetrahydr...	370	C21H38O5	1000329-87-0	38
5			Octanamide, N-methallyl-	197	C12H23NO	1000340-16-1	35



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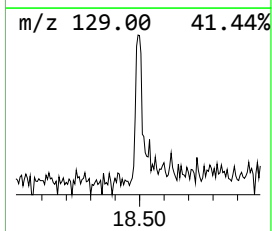
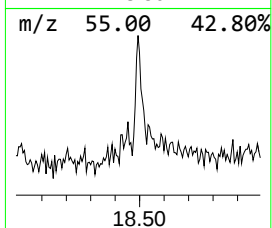
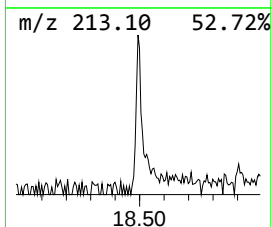
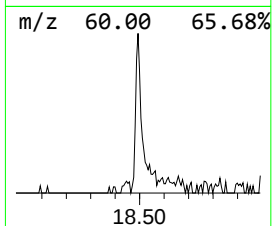
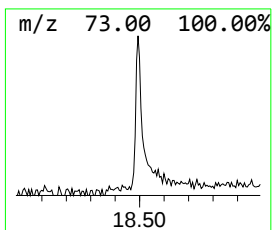
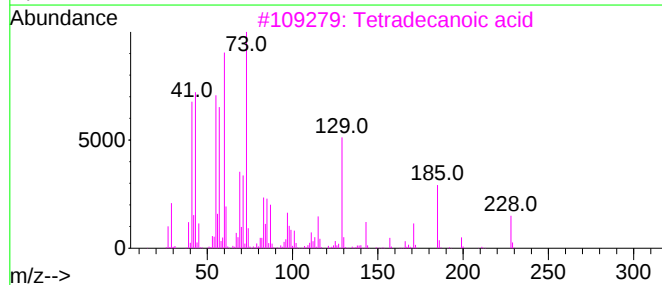
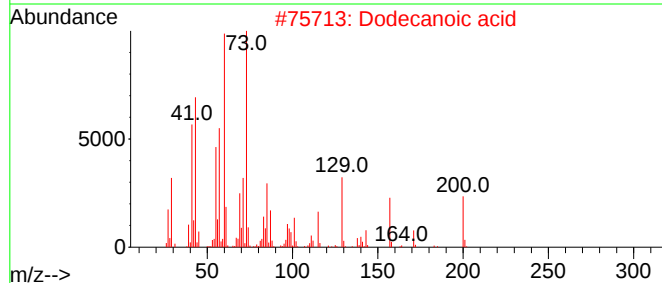
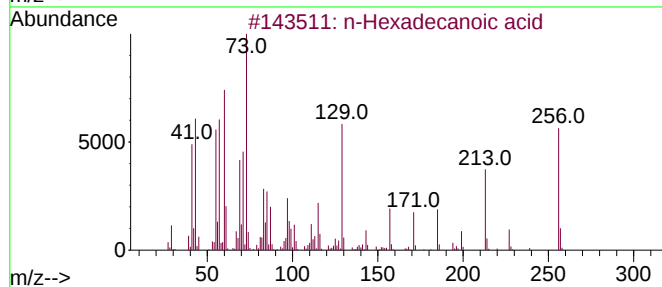
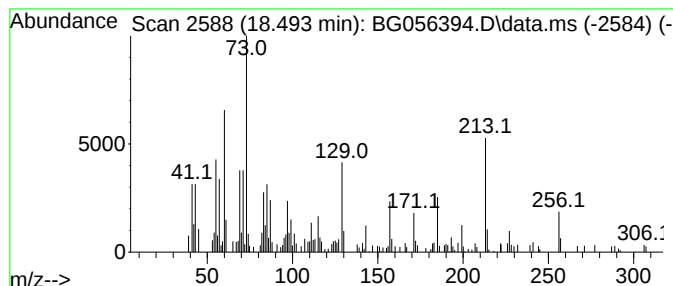
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.493	3.81 ng	138796	Phenanthrene-d10	17.647

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2			Dodecanoic acid	200	C12H24O2	000143-07-7	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4			Tridecanoic acid	214	C13H26O2	000638-53-9	60
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.332	6.4	ng	87128	1	8.299	271225	20.0
Benzophenone	16.249	2.0	ng	62571	3	14.909	614442	20.0
Sulfurous acid,...	16.596	2.3	ng	83143	4	17.647	728883	20.0
n-Hexadecanoic ...	18.493	3.8	ng	138796	4	17.647	728883	20.0