

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
 Data File : BG055165.D
 Acq On : 13 Oct 2022 15:50
 Operator : CG/JU
 Sample : N5105-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-5

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-BG101322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055165.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.326	3	6	13	rVB	285810	368927	24.56%	3.764%
2	3.884	95	101	114	rBV	158536	242622	16.15%	2.476%
3	5.341	343	349	357	rVB	108361	164864	10.98%	1.682%
4	5.823	422	431	439	rBV	438154	723421	48.16%	7.381%
5	7.433	697	705	715	rBV	476385	809899	53.92%	8.264%
6	8.302	846	853	864	rBV	131709	226080	15.05%	2.307%
7	9.471	1044	1052	1061	rBV	286381	500459	33.32%	5.106%
8	10.876	1285	1291	1300	rVB2	11908	20037	1.33%	0.204%
9	11.134	1327	1335	1343	rBV	191426	345215	22.98%	3.522%
10	13.543	1738	1745	1751	rBV	742282	1117991	74.43%	11.408%
11	14.348	1877	1882	1889	rBV	9816	15045	1.00%	0.154%
12	14.912	1969	1978	1985	rVB	321286	502997	33.49%	5.132%
13	16.387	2222	2229	2240	rBV	609329	932208	62.06%	9.512%
14	17.644	2436	2443	2449	rBV	380709	590309	39.30%	6.023%
15	18.496	2583	2588	2596	rBV3	32783	52700	3.51%	0.538%
16	19.748	2797	2801	2806	rBV6	14554	25090	1.67%	0.256%
17	20.212	2875	2880	2886	rBV	1095732	1502099	100.00%	15.327%
18	20.506	2926	2930	2933	rVB4	14530	18200	1.21%	0.186%
19	21.005	3010	3015	3018	rBV3	18326	26340	1.75%	0.269%
20	21.528	3099	3104	3110	rBV	75727	121525	8.09%	1.240%
21	21.922	3162	3171	3180	rBV	378073	664235	44.22%	6.778%
22	22.104	3198	3202	3207	rVB	17503	27126	1.81%	0.277%
23	22.744	3308	3311	3315	rBV3	15657	24924	1.66%	0.254%
24	23.461	3428	3433	3443	rVB6	33468	96694	6.44%	0.987%
25	25.341	3743	3753	3766	rVB2	211608	681463	45.37%	6.953%

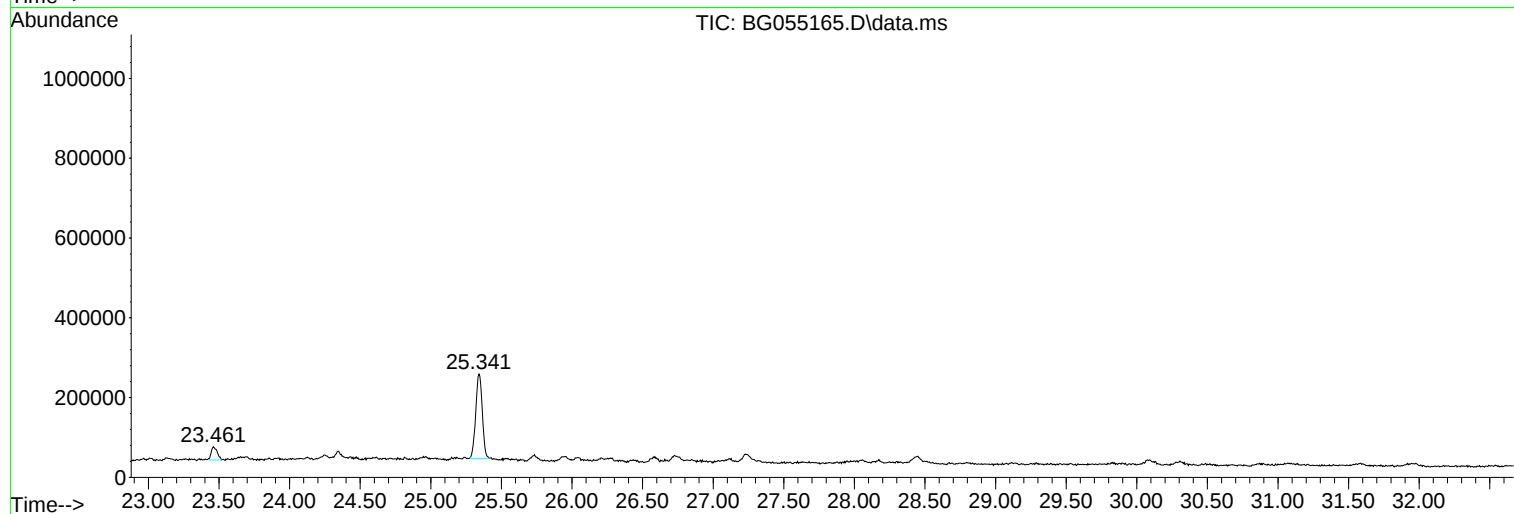
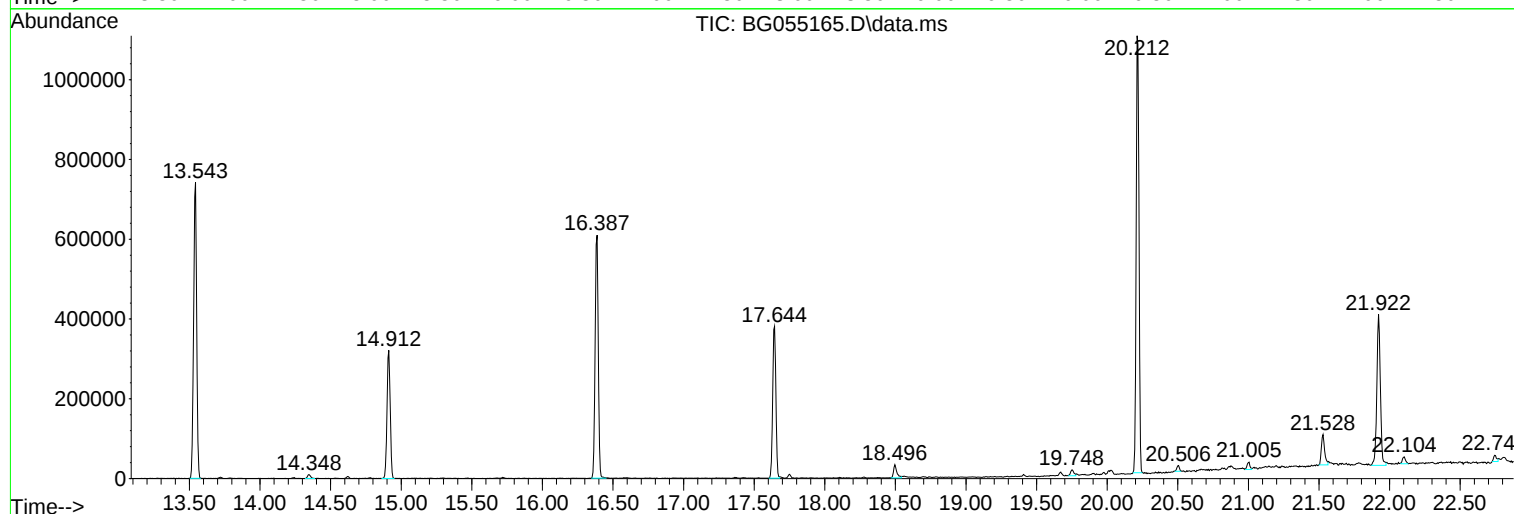
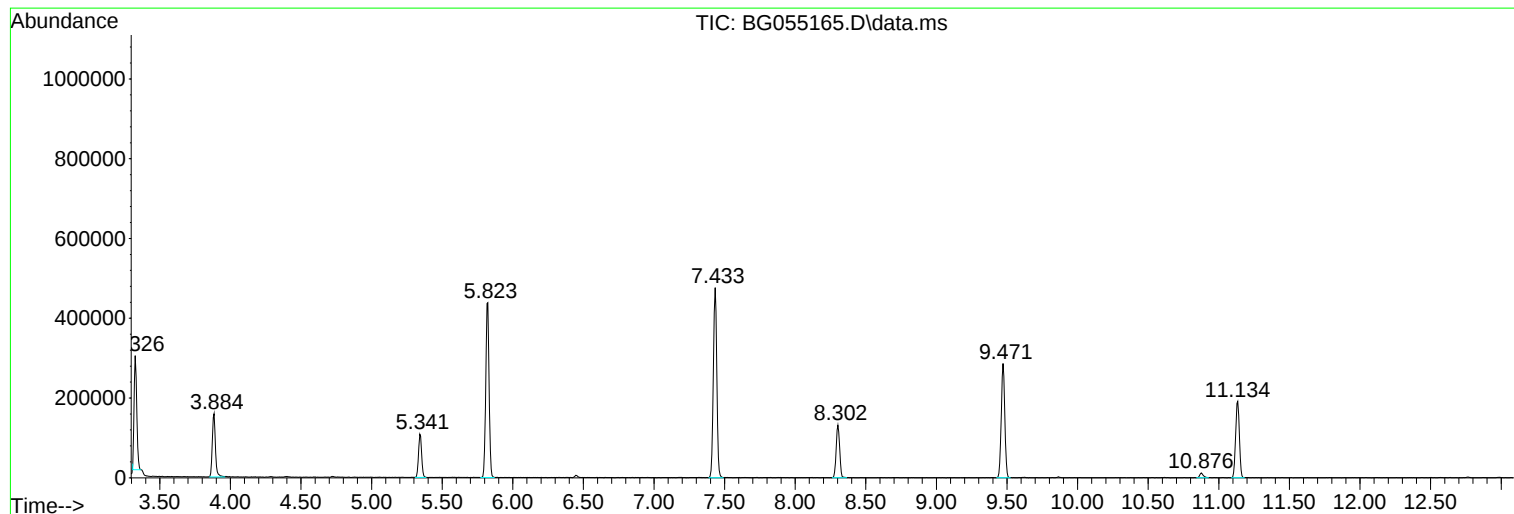
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG055165.D
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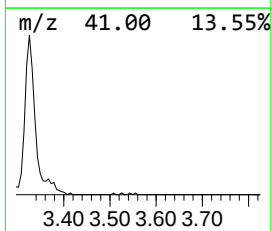
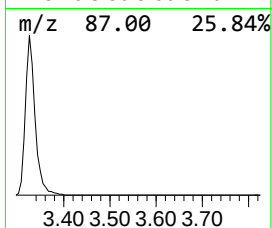
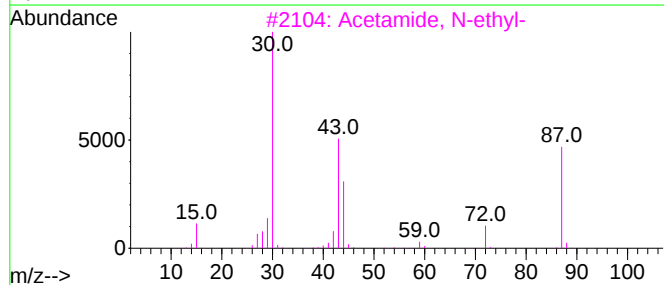
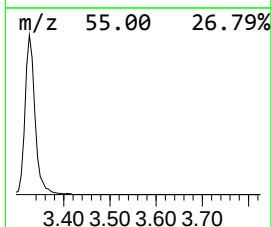
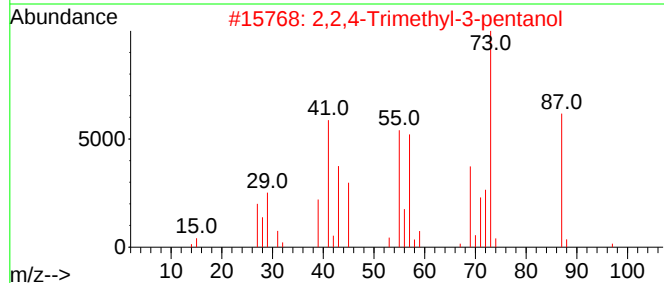
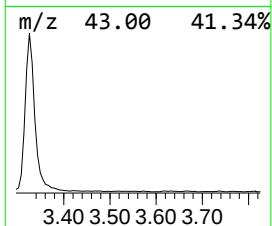
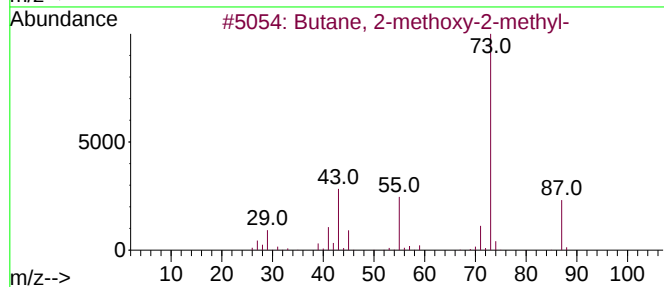
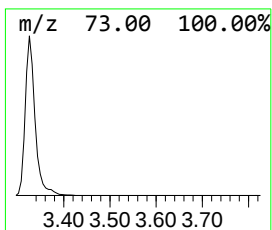
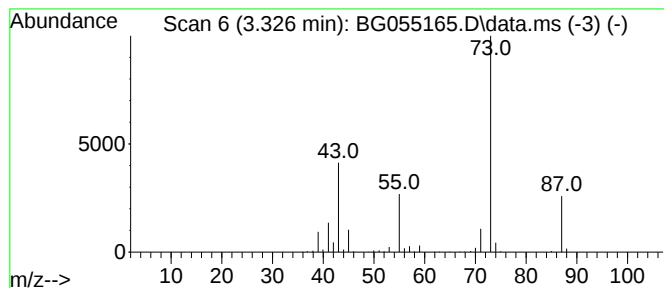
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
3.326	32.64 ng	368927	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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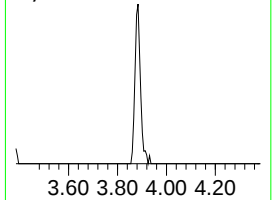
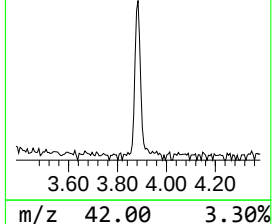
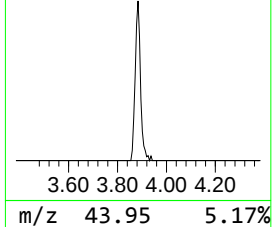
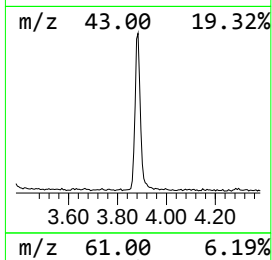
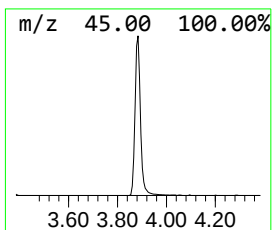
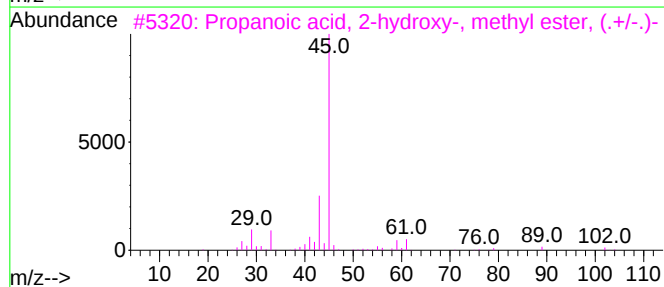
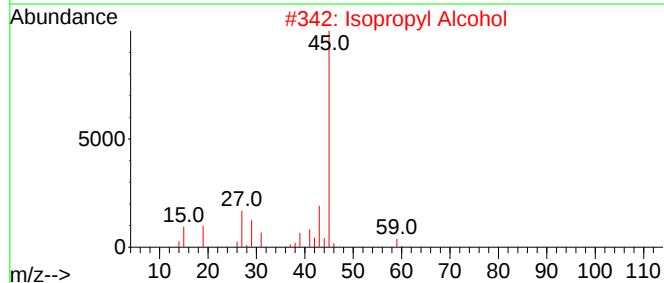
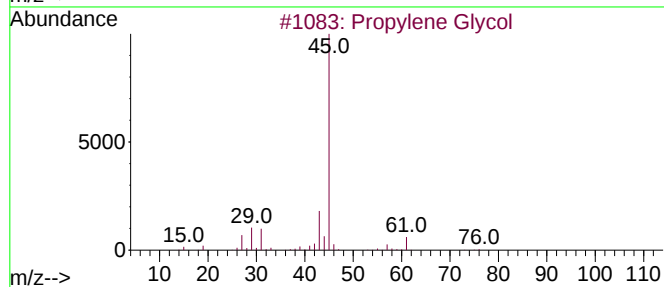
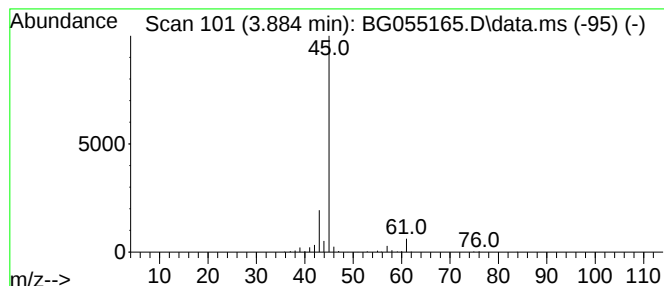
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.884	21.46 ng	242622	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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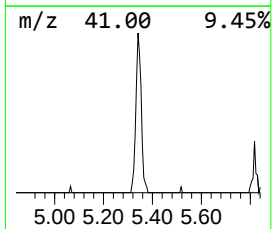
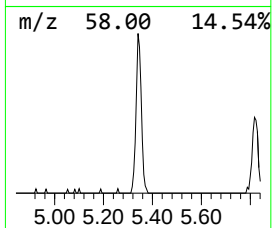
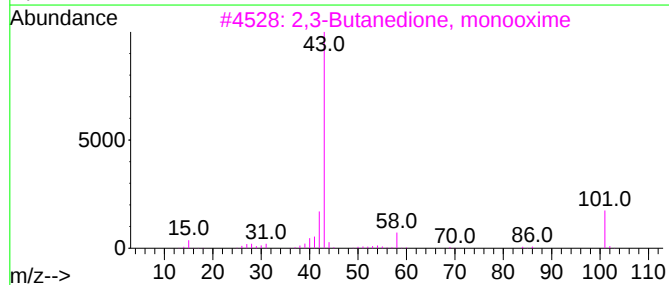
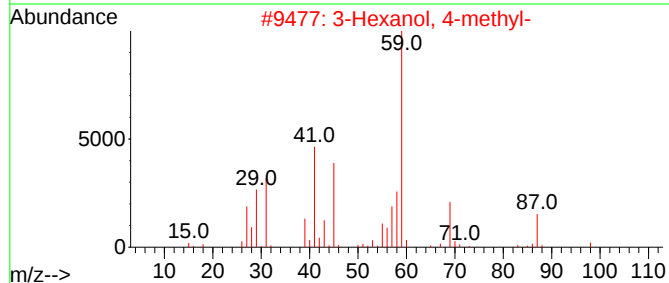
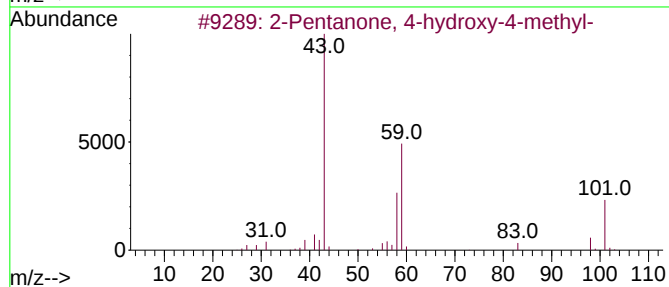
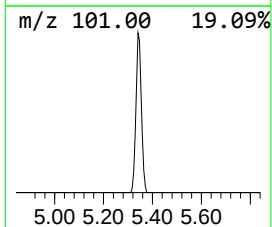
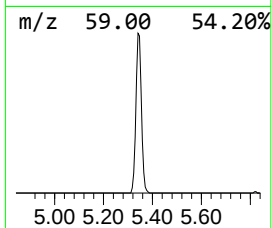
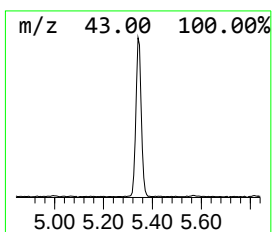
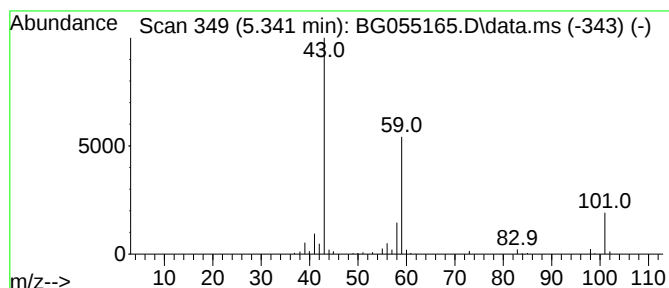
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.341	14.58 ng	164864	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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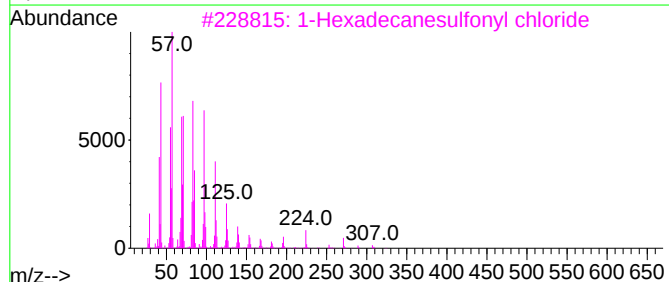
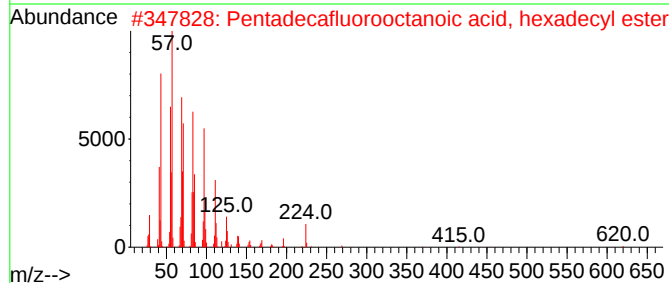
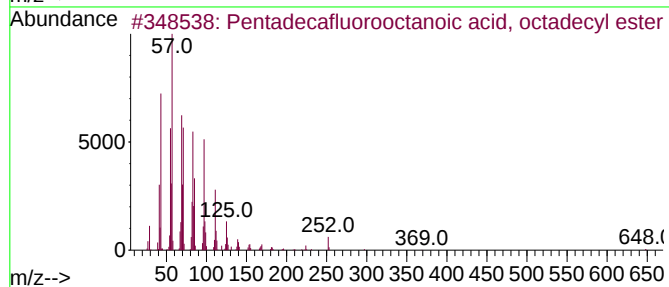
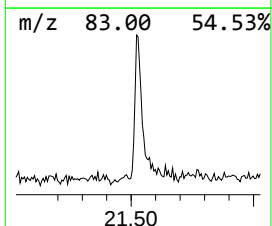
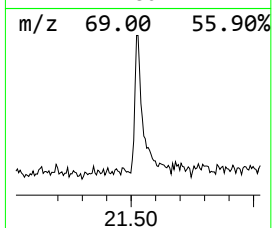
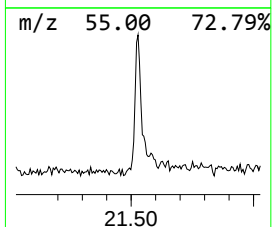
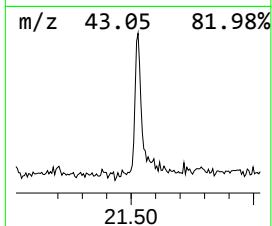
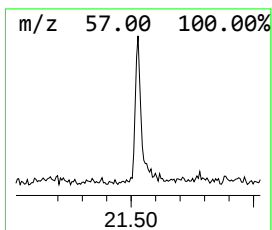
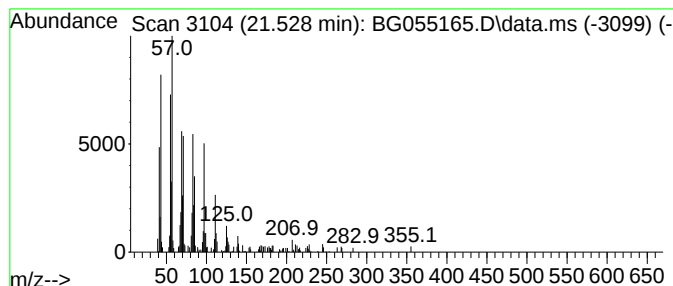
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.528	3.66 ng	121525	Chrysene-d12	21.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



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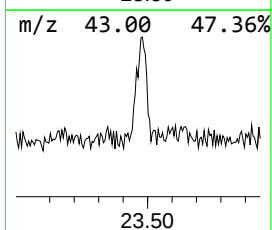
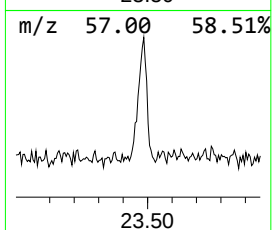
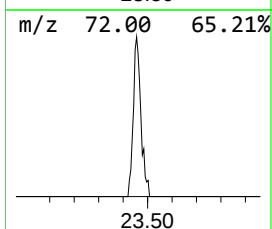
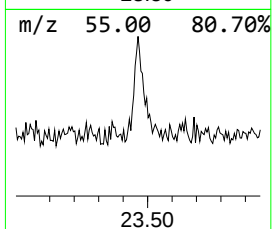
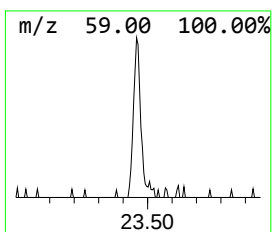
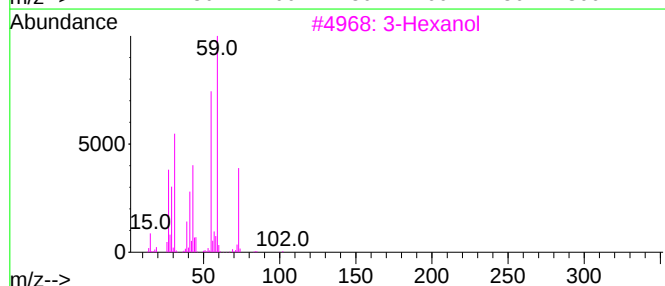
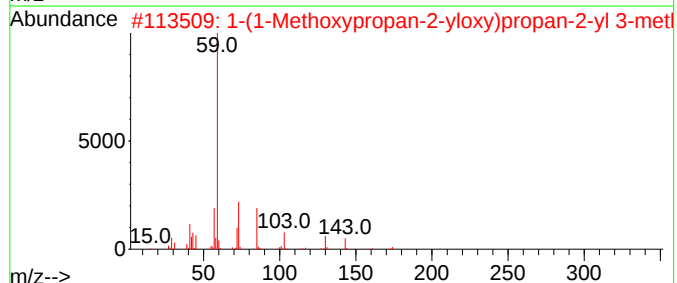
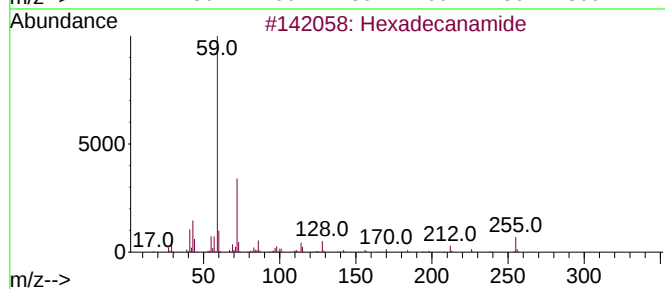
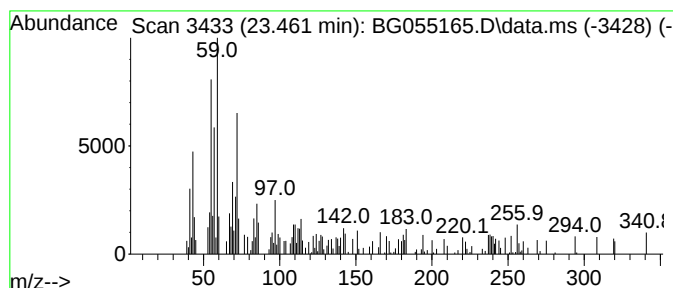
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.461	2.91 ng	96694	Chrysene-d12	21.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanamide	255	C16H33NO	000629-54-9	52
2			1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	35
3			3-Hexanol	102	C6H14O	000623-37-0	27
4			Propanedioic acid, diazo-, dimet...	158	C5H6N2O4	006773-29-1	27
5			But-3-enoylamide, 3-methyl-N-pro...	225	C14H27NO	1000437-83-2	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.326	32.6	ng	368927	1	8.302	226080	20.0
Propylene Glycol	3.884	21.5	ng	242622	1	8.302	226080	20.0
2-Pentanone, 4-...	5.341	14.6	ng	164864	1	8.302	226080	20.0
Pentadecafluoro...	21.528	3.7	ng	121525	5	21.922	664235	20.0
Hexadecanamide	23.461	2.9	ng	96694	5	21.922	664235	20.0