

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
 Data File : BG057493.D
 Acq On : 22 May 2023 14:30
 Operator : CG/JU
 Sample : 02845-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP1

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.389	309	315	323	rBB	19112	30259	2.53%	0.495%
2	5.877	391	398	409	rBB	244815	402418	33.66%	6.584%
3	7.498	667	674	684	rBV	256619	456028	38.14%	7.461%
4	8.356	812	820	828	rBB	63277	109760	9.18%	1.796%
5	9.536	1014	1021	1031	rBV	158820	283181	23.68%	4.633%
6	11.199	1295	1304	1310	rBV	88984	156300	13.07%	2.557%
7	13.596	1704	1712	1720	rBV	469531	725588	60.69%	11.872%
8	14.917	1931	1937	1941	rBV	91741	133526	11.17%	2.185%
9	14.976	1941	1947	1957	rVB	147439	244741	20.47%	4.004%
10	15.199	1981	1985	1990	rBV3	12804	16592	1.39%	0.271%
11	15.276	1991	1998	2003	rBV3	11061	16192	1.35%	0.265%
12	16.309	2164	2174	2181	rBV	67138	107201	8.97%	1.754%
13	16.415	2187	2192	2194	rBV2	11383	15469	1.29%	0.253%
14	16.456	2194	2199	2206	rVB	403353	597252	49.95%	9.772%
15	16.791	2252	2256	2265	rBV4	19145	31805	2.66%	0.520%
16	16.873	2265	2270	2280	rVB3	10117	15684	1.31%	0.257%
17	17.713	2405	2413	2418	rBV	216148	321276	26.87%	5.257%
18	17.755	2418	2420	2425	rVB	13633	17762	1.49%	0.291%
19	18.577	2553	2560	2565	rBV6	6732	19224	1.61%	0.315%
20	19.746	2755	2759	2764	rVB	20809	27896	2.33%	0.456%
21	20.104	2816	2820	2827	rVB	16906	23413	1.96%	0.383%
22	20.281	2844	2850	2856	rBV	966007	1195632	100.00%	19.563%
23	21.238	3009	3013	3016	rVB6	11098	16246	1.36%	0.266%
24	21.414	3038	3043	3049	rVB	256923	367090	30.70%	6.006%
25	21.579	3066	3071	3078	rBV2	34729	73045	6.11%	1.195%
26	22.019	3140	3146	3154	rBV2	194768	343538	28.73%	5.621%
27	23.541	3402	3405	3413	rVB9	6991	12410	1.04%	0.203%
28	24.410	3547	3553	3557	rBV6	10696	22896	1.91%	0.375%
29	25.521	3733	3742	3754	rVB2	105412	329403	27.55%	5.390%

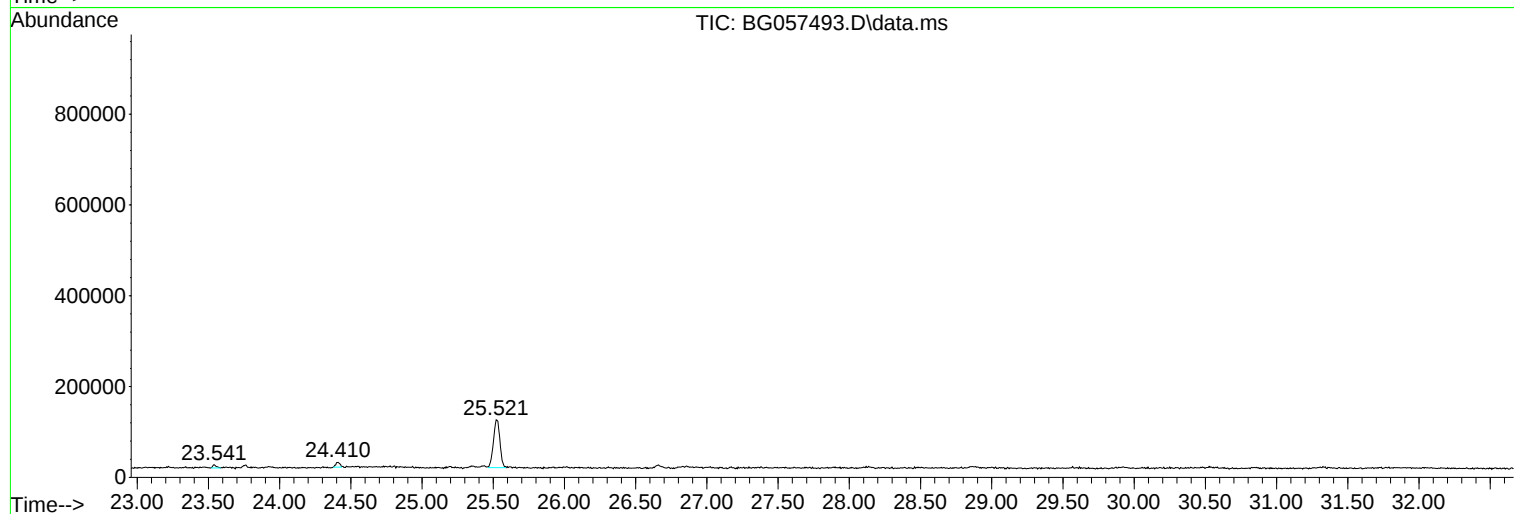
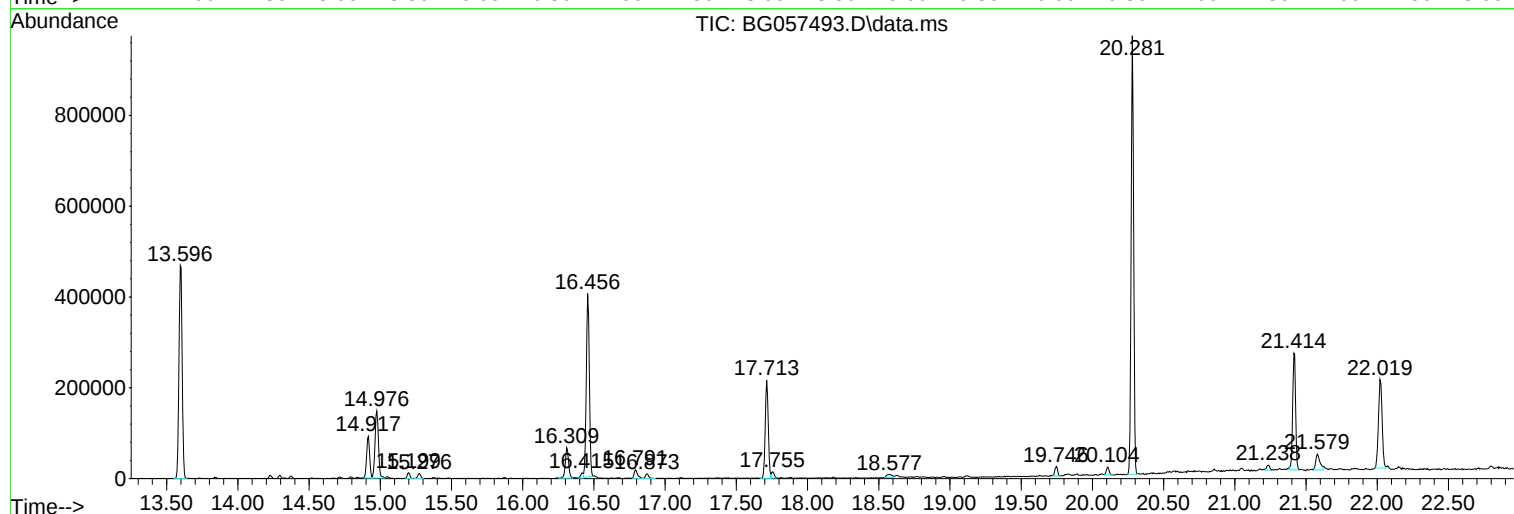
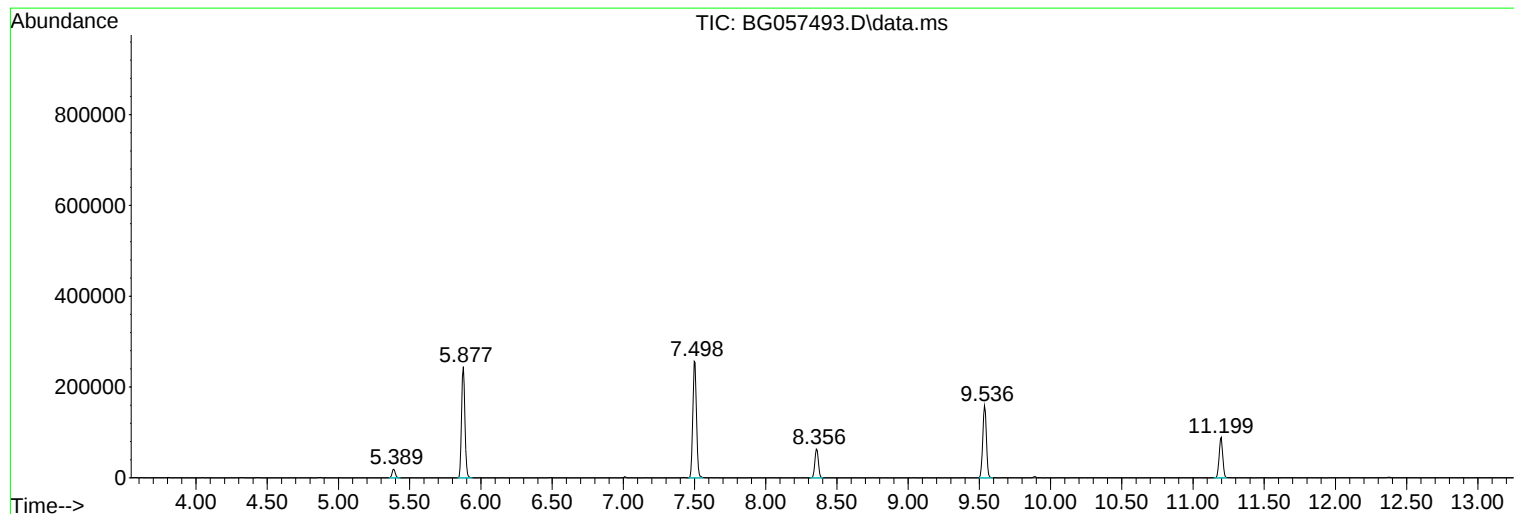
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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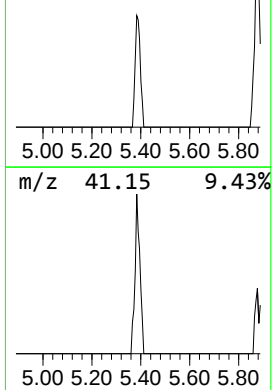
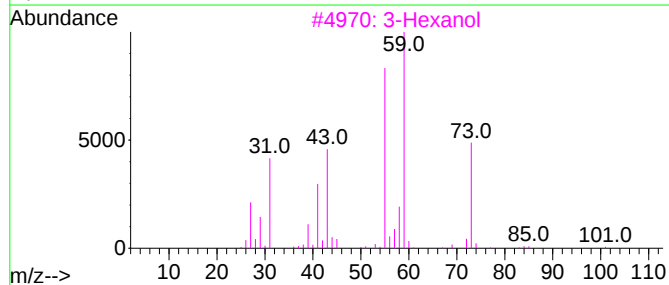
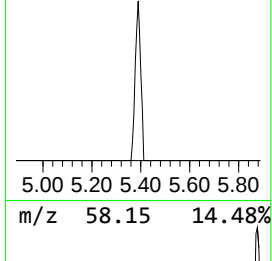
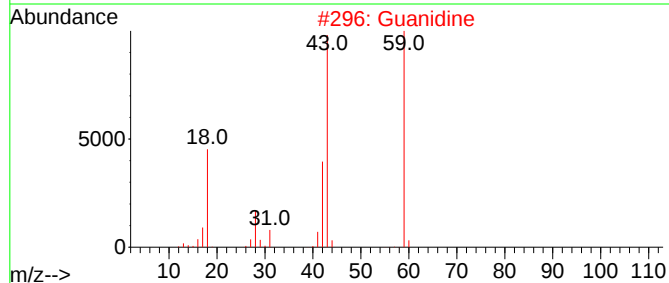
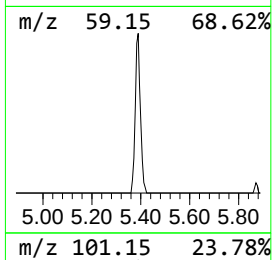
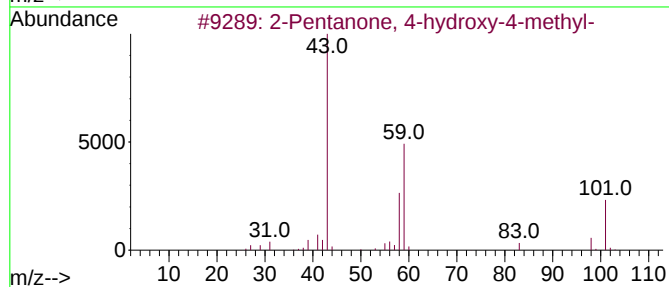
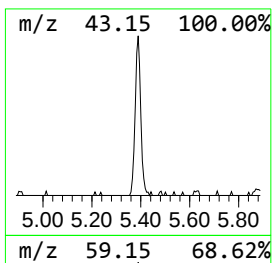
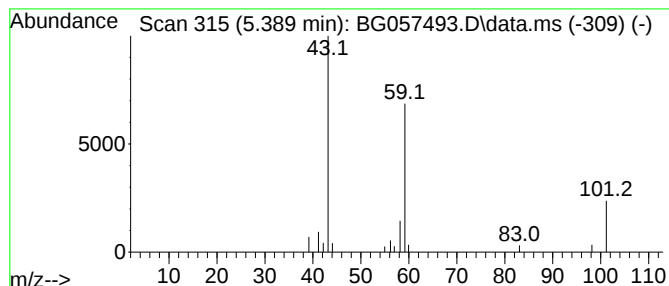
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.389	5.51 ng	30259	1,4-Dichlorobenzene-d4	8.356

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Guanidine	59	CH5N3	000113-00-8	47	
3	3-Hexanol	102	C6H14O	000623-37-0	33	
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32	
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23	



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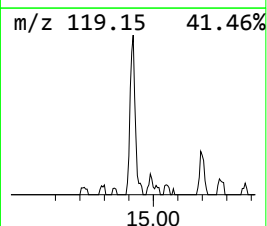
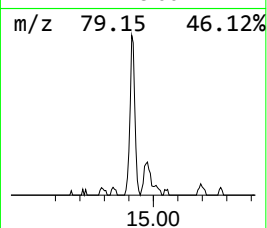
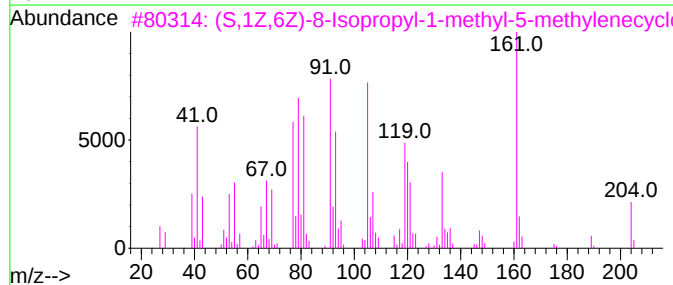
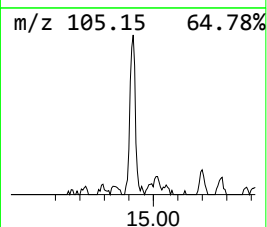
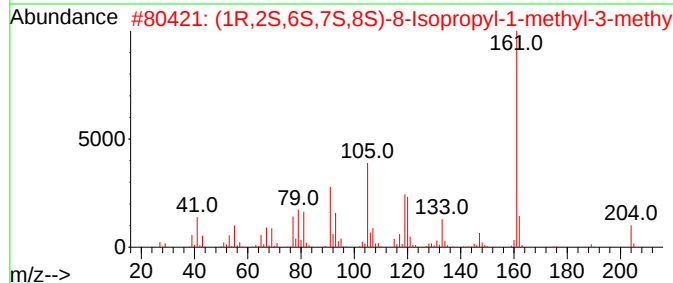
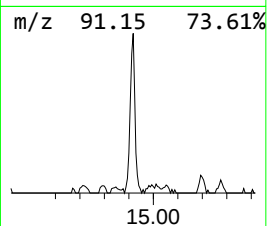
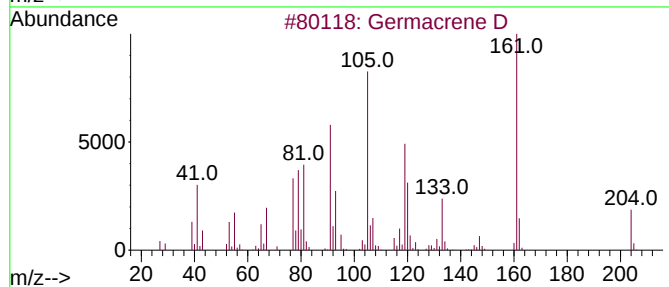
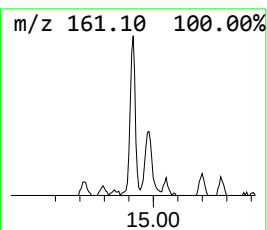
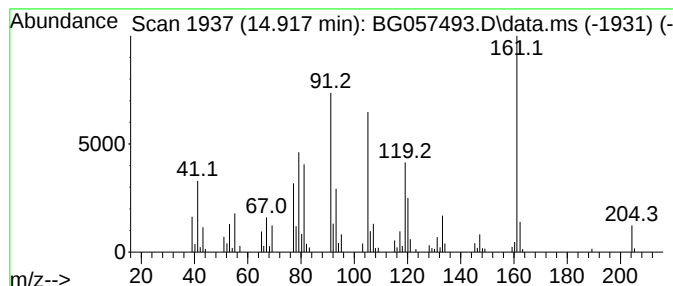
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Germacrene D Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.917	10.91 ng	133526	Acenaphthene-d10	14.976

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germacrene D	204	C15H24	023986-74-5	98
2			(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	97
3			(S,1Z,6Z)-8-Isopropyl-1-methyl-5...	204	C15H24	317819-80-0	95
4			(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	94
5			1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	94



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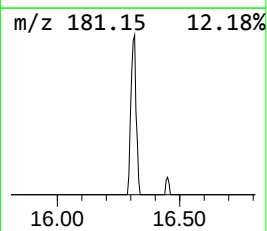
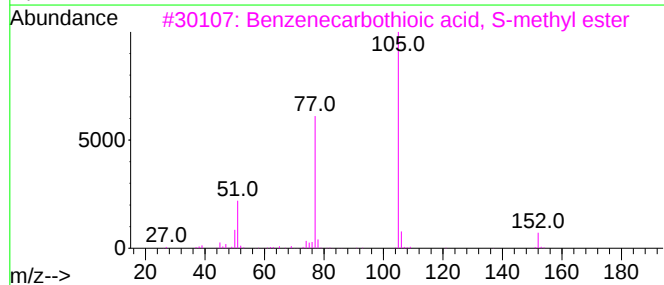
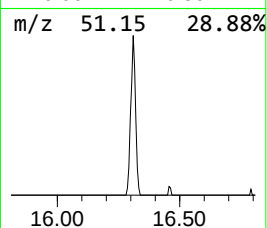
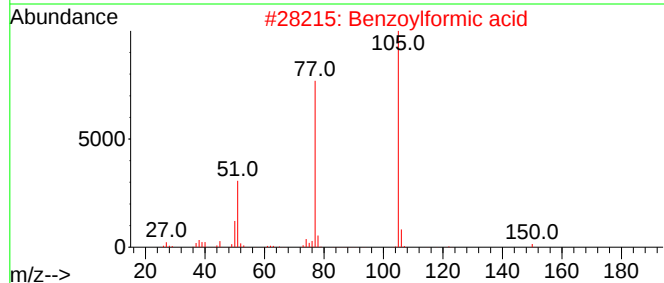
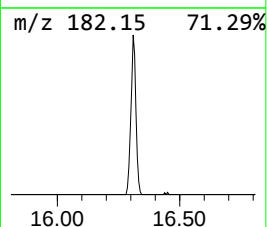
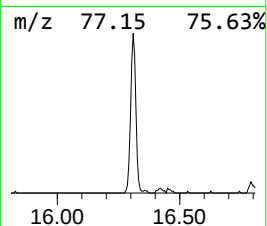
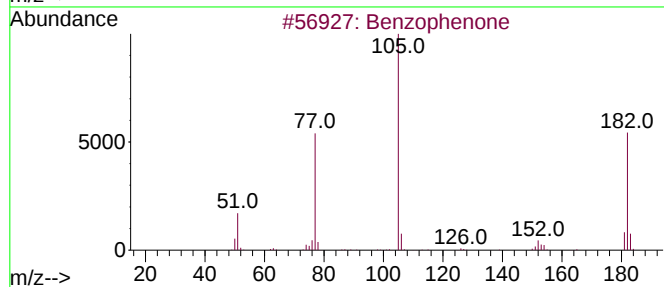
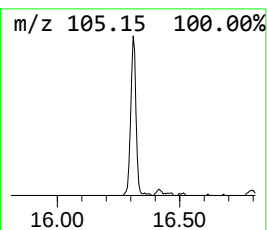
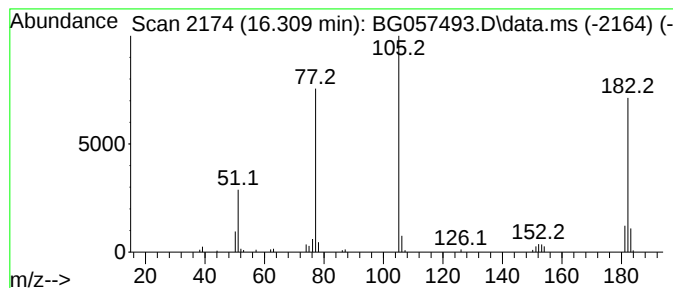
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	8.76 ng	107201	Acenaphthene-d10	14.976

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzoylformic acid	150	C8H6O3	000611-73-4	53
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
5			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	50



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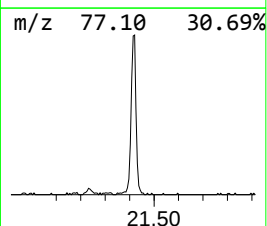
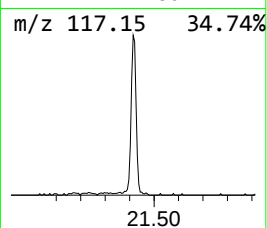
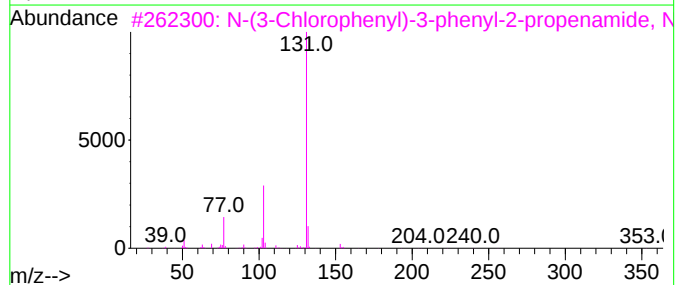
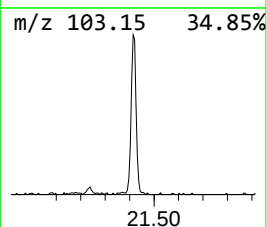
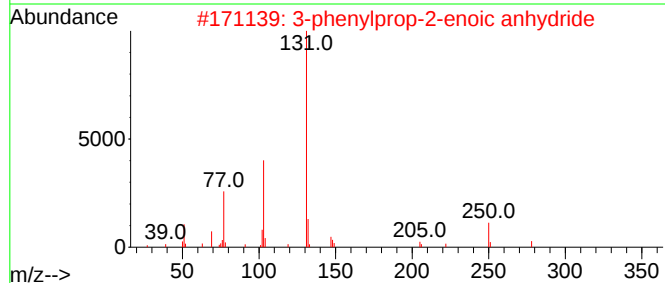
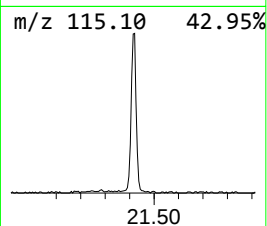
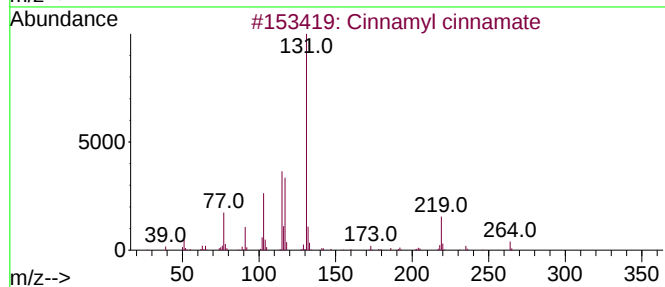
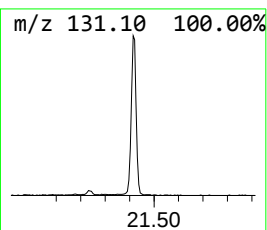
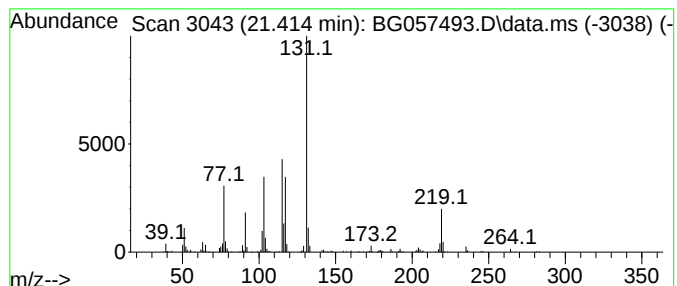
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.414	21.37 ng	367090	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	47
3			N-(3-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-37-1	47
4			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
5			N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47



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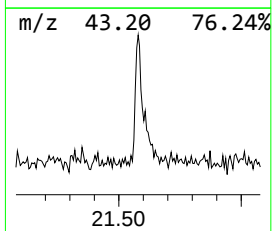
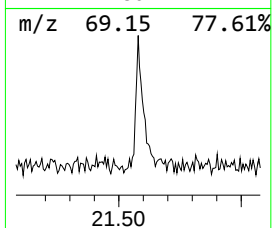
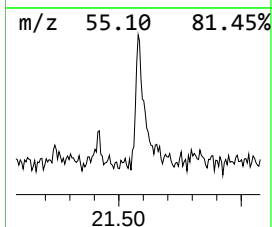
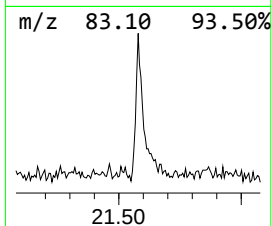
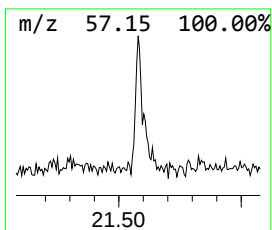
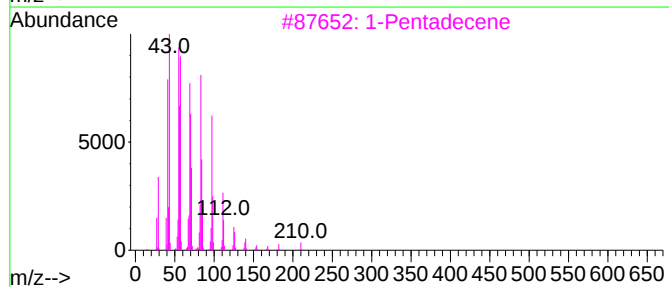
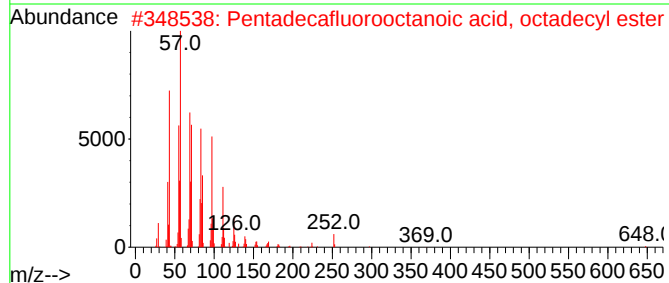
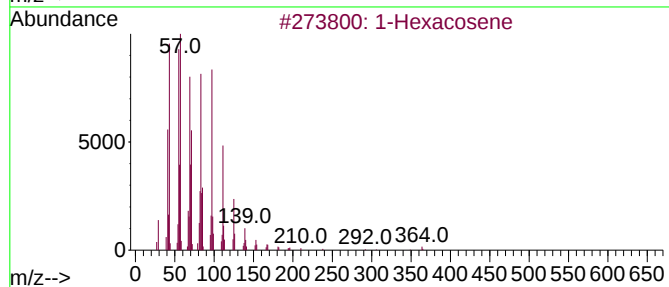
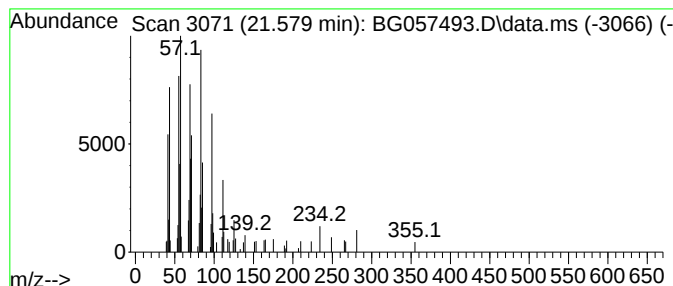
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Peak Number 5 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.579	4.25 ng	73045	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	90
2	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	87
3	1-Pentadecene			210	C15H30	013360-61-7	86
4	1-Octadecanol			270	C18H38O	000112-92-5	81
5	Pentadecafluorooctanoic acid, pe...			624	C23H31F15O2	1000406-04-5	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.389	5.5	ng	30259	1	8.356	109760	20.0
Germacrene D	14.917	10.9	ng	133526	3	14.976	244741	20.0
Benzophenone	16.310	8.8	ng	107201	3	14.976	244741	20.0
Cinnamyl cinnamate	21.414	21.4	ng	367090	5	22.019	343538	20.0
1-Hexacosene	21.579	4.3	ng	73045	5	22.019	343538	20.0