

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
 Data File : BG057799.D
 Acq On : 22 Jun 2023 00:58
 Operator : CG/JU
 Sample : 03302-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-2

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.030	323	330	339	rVB	414355	616407	31.75%	6.041%
2	5.488	402	408	416	rBV	403380	643819	33.16%	6.309%
3	7.080	671	679	687	rBV	451870	749781	38.61%	7.348%
4	7.921	816	822	828	rBV	111918	181994	9.37%	1.783%
5	9.078	1011	1019	1027	rBV	249413	435962	22.45%	4.272%
6	10.723	1290	1299	1310	rBB	166872	285711	14.71%	2.800%
7	13.179	1710	1717	1724	rBV	678527	1017022	52.38%	9.966%
8	14.554	1942	1951	1960	rVB	286682	432546	22.28%	4.239%
9	15.911	2176	2182	2188	rBV	49422	71386	3.68%	0.700%
10	16.040	2197	2204	2211	rBV	659162	974156	50.17%	9.546%
11	17.298	2411	2418	2428	rVB	431524	638919	32.90%	6.261%
12	18.185	2564	2569	2578	rBV3	34877	59258	3.05%	0.581%
13	19.918	2857	2864	2869	rBV	1456160	1941724	100.00%	19.028%
14	21.164	3071	3076	3079	rBV2	19913	38188	1.97%	0.374%
15	21.205	3079	3083	3092	rVV4	168446	280406	14.44%	2.748%
16	21.287	3092	3097	3104	rVB	98011	141817	7.30%	1.390%
17	21.552	3136	3142	3148	rVB	427119	683544	35.20%	6.698%
18	21.751	3172	3176	3182	rBV	25276	36556	1.88%	0.358%
19	22.357	3273	3279	3290	rVB6	23834	55442	2.86%	0.543%
20	23.026	3389	3393	3400	rVB3	16372	26745	1.38%	0.262%
21	23.209	3422	3424	3433	rVB2	16423	27821	1.43%	0.273%
22	24.701	3667	3678	3692	rBV	278663	791788	40.78%	7.759%
23	25.970	3888	3894	3906	rVB5	25767	73469	3.78%	0.720%

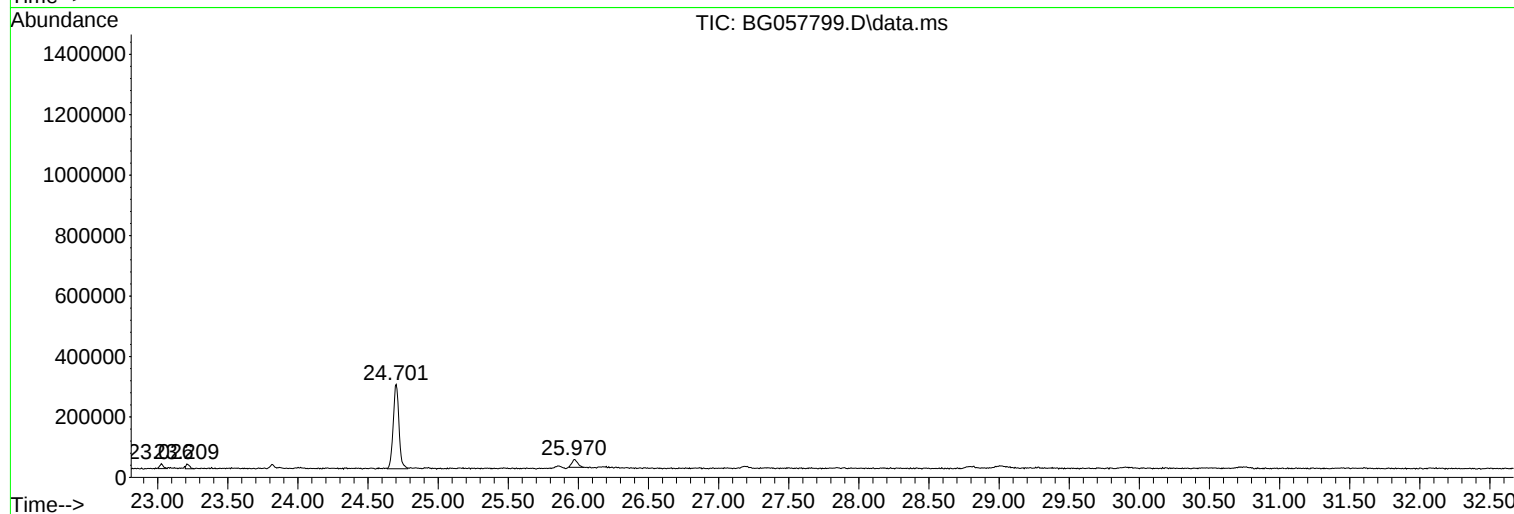
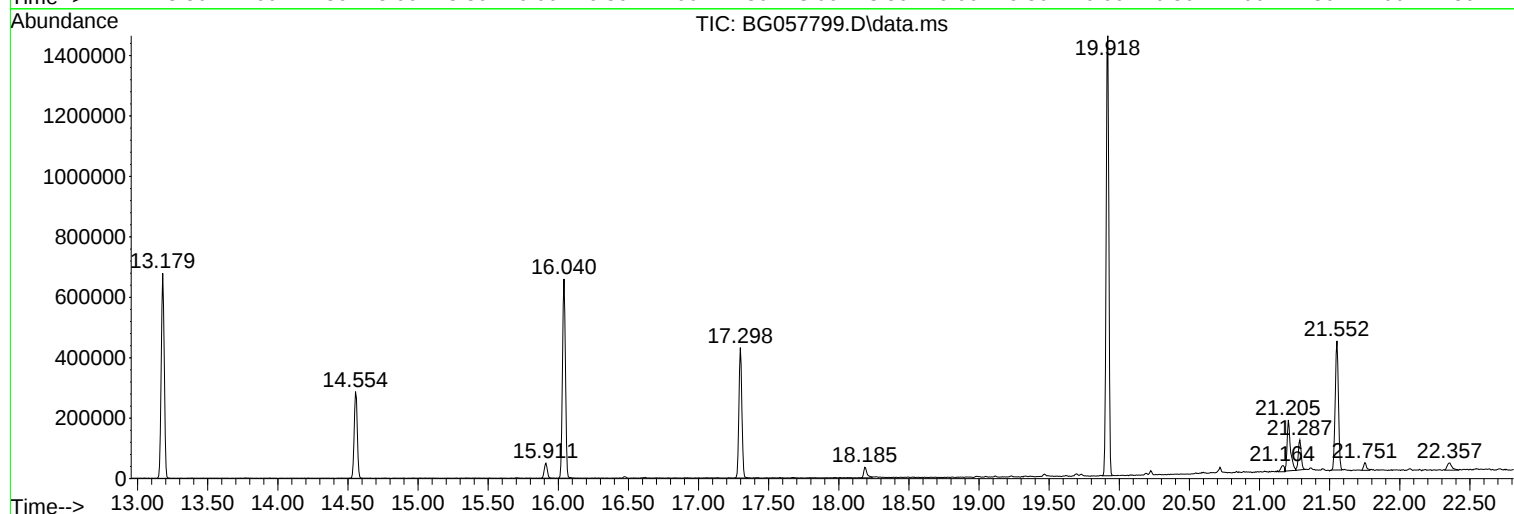
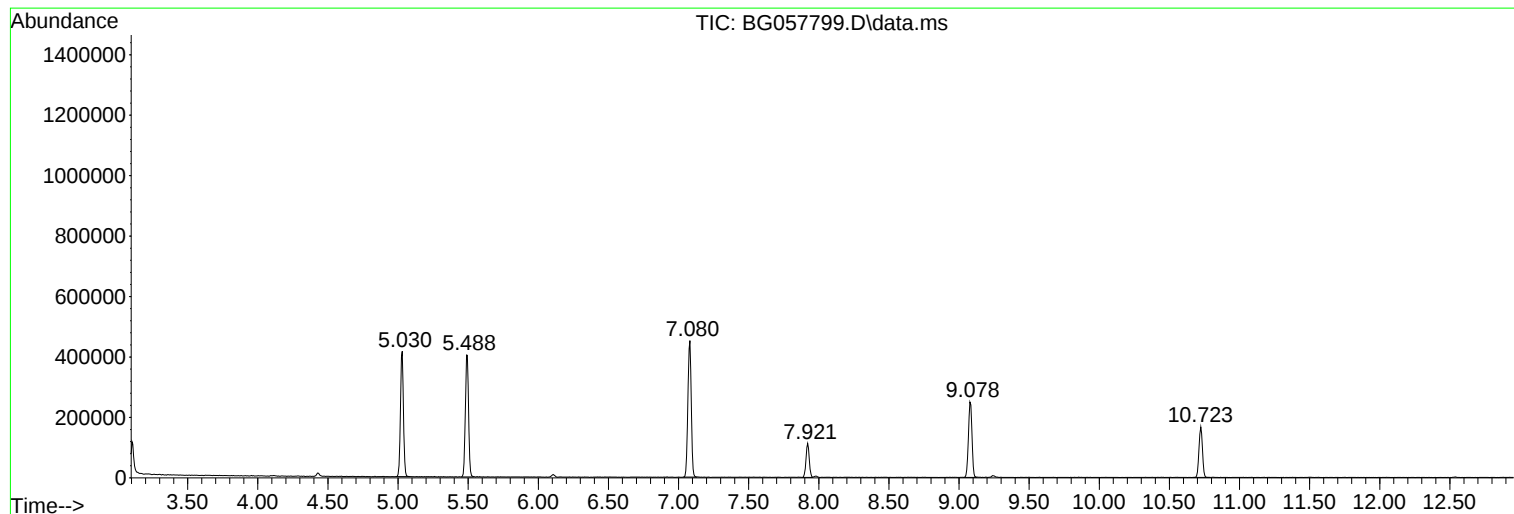
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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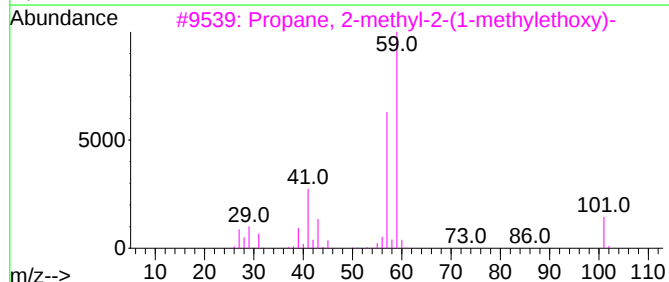
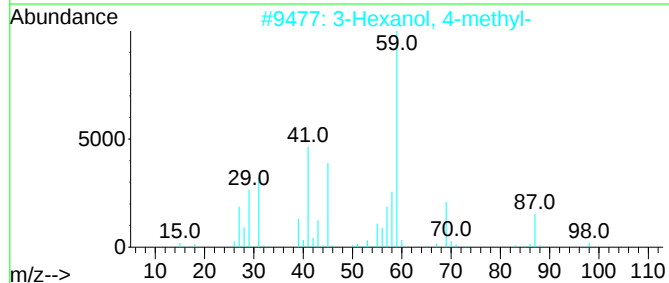
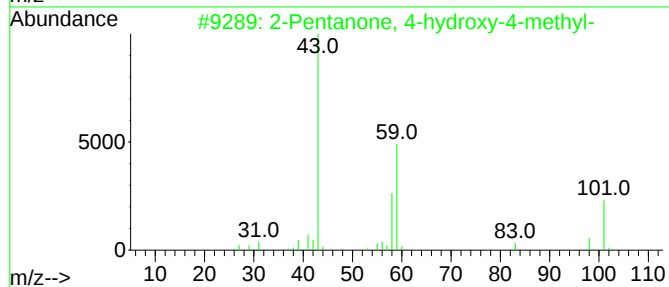
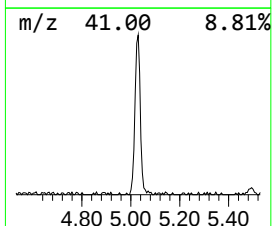
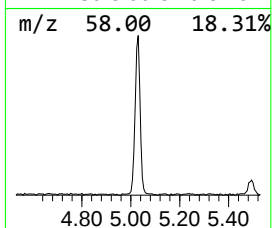
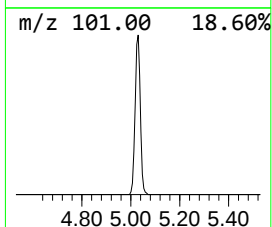
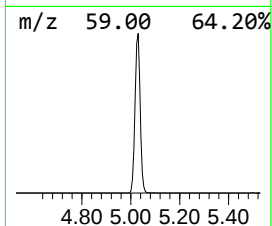
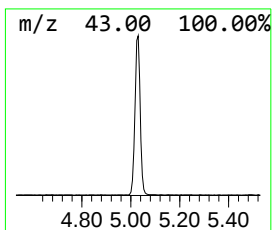
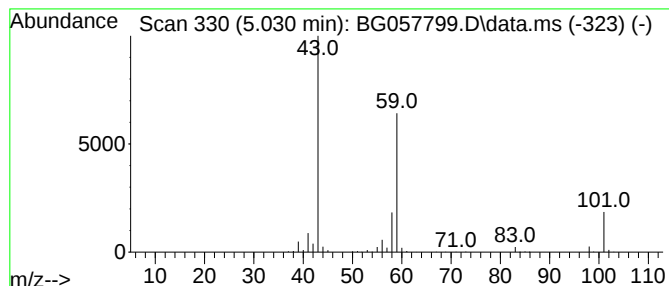
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.030	67.74 ng	616407	1,4-Dichlorobenzene-d4	7.921

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	33		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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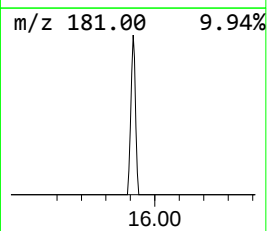
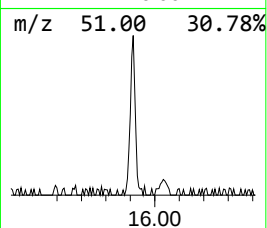
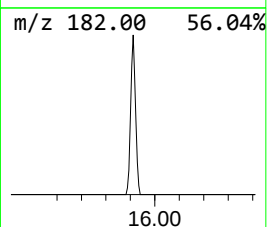
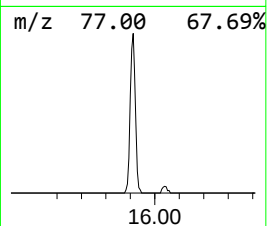
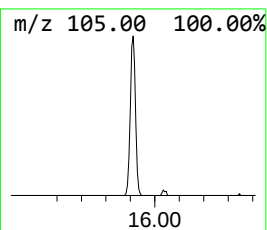
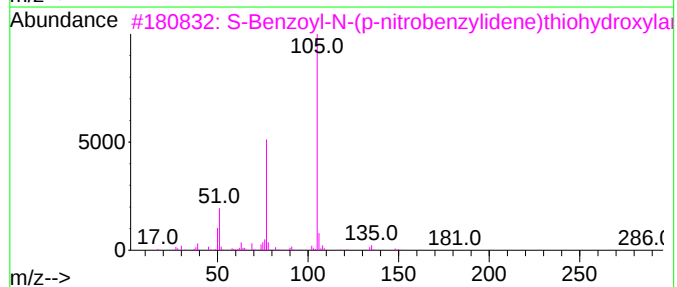
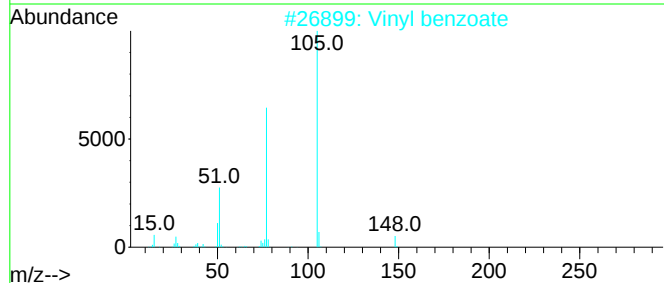
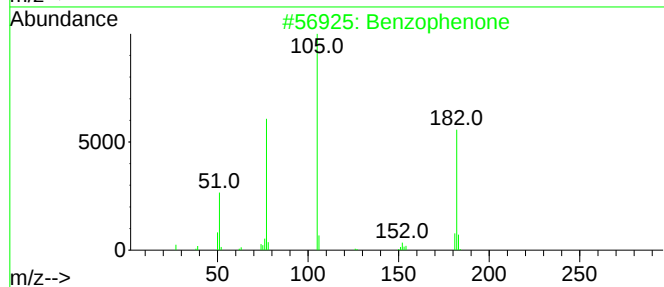
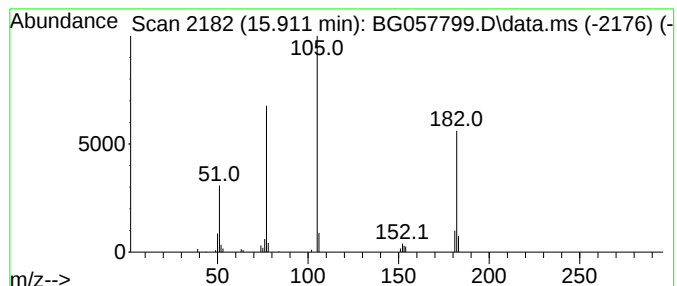
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	3.30 ng	71386	Acenaphthene-d10	14.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Vinyl benzoate	148	C9H8O2	000769-78-8	47
3			S-Benzoyl-N-(p-nitrobenzylidene)...	286	C14H10N2O3S	139776-09-3	47
4			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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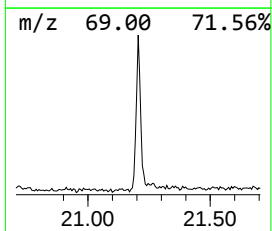
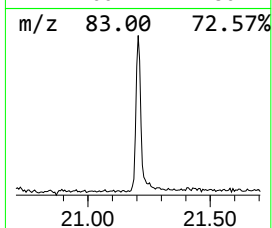
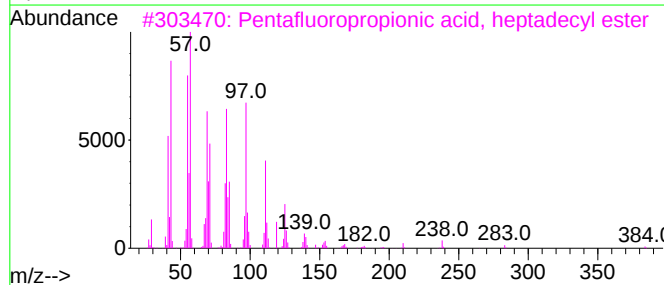
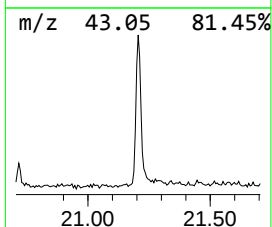
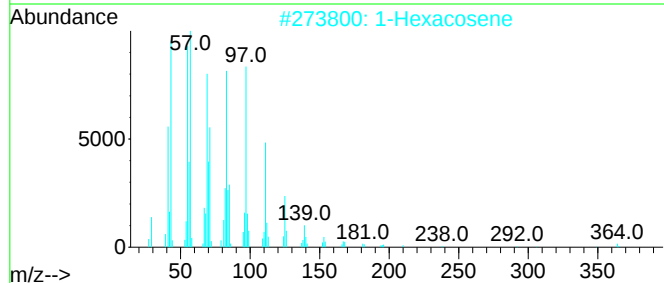
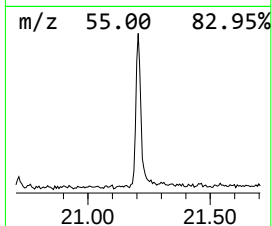
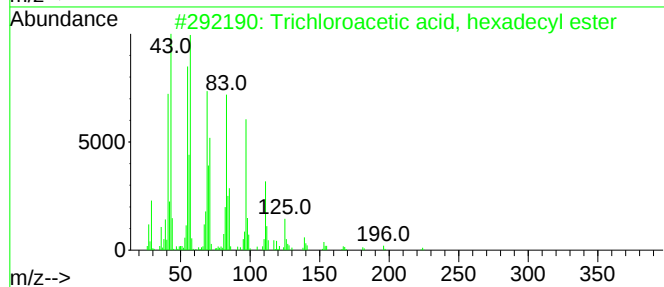
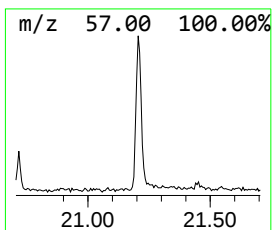
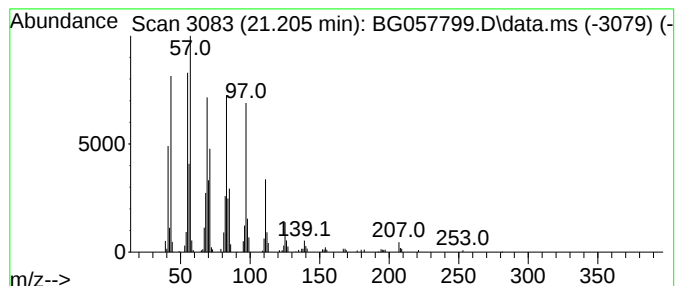
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Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	8.20 ng	280406	Chrysene-d12	21.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



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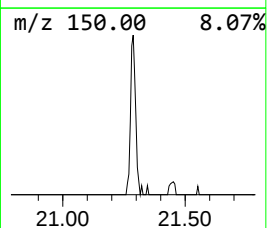
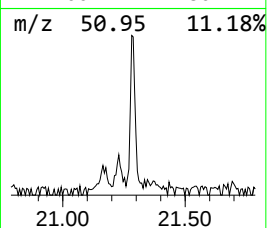
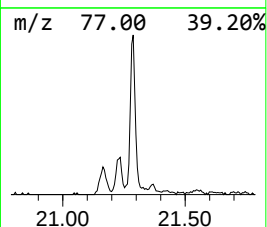
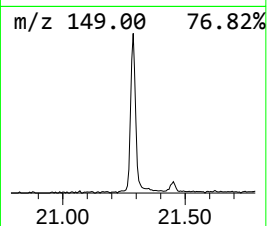
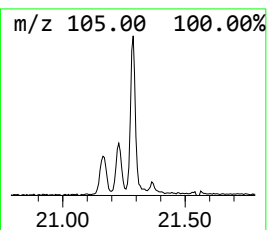
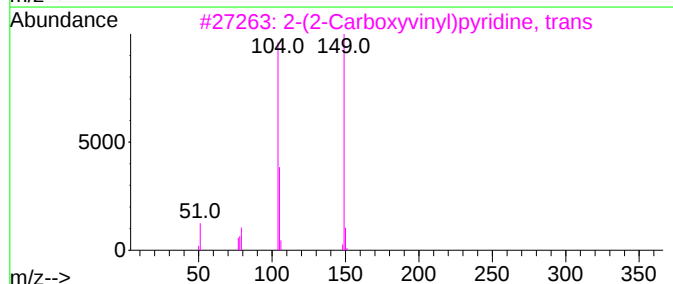
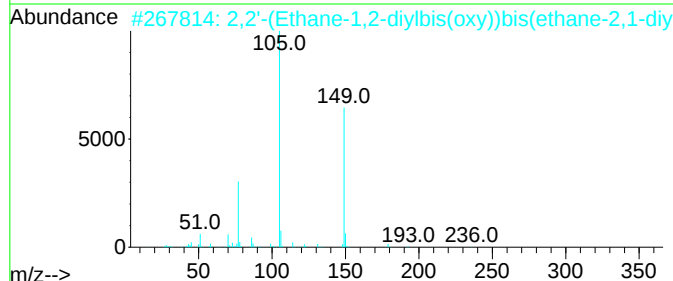
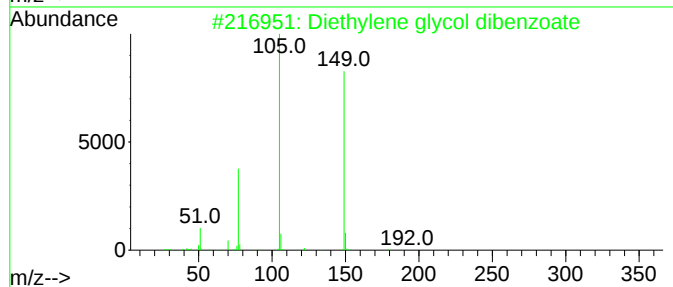
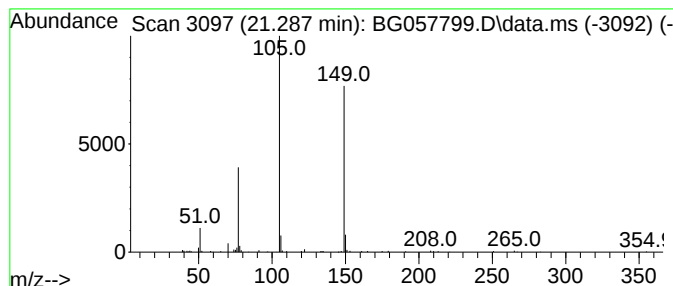
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.287	4.15 ng	141817	Chrysene-d12	21.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			N-(2-Fluoro-5-nitrophenyl)benzamide	260	C13H9FN2O3	144205-37-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.030	67.7	ng	616407	1	7.921	181994	20.0
Benzophenone	15.911	3.3	ng	71386	3	14.554	432546	20.0
Trichloroacetic...	21.205	8.2	ng	280406	5	21.552	683544	20.0
Diethylene glyc...	21.287	4.2	ng	141817	5	21.552	683544	20.0