

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
 Data File : BG054942.D
 Acq On : 14 Sep 2022 13:57
 Operator : CG/JU
 Sample : N4579-23
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHERRY-HILL-COMP-16

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	319	324	330	rBV	22726	36044	2.09%	0.394%
2	5.673	399	406	418	rBV	420240	676457	39.31%	7.391%
3	7.289	673	681	696	rBV	413388	727718	42.28%	7.952%
4	8.135	818	825	833	rBV	112434	196901	11.44%	2.151%
5	9.310	1017	1025	1034	rBV	242807	451697	26.25%	4.936%
6	10.709	1258	1263	1273	rBV	17678	39608	2.30%	0.433%
7	10.961	1296	1306	1313	rBV	162858	299550	17.41%	3.273%
8	13.394	1712	1720	1728	rBV	783062	1210579	70.34%	13.228%
9	14.769	1946	1954	1964	rBV	295866	476131	27.67%	5.203%
10	16.261	2201	2208	2219	rBV	586319	944978	54.91%	10.325%
11	16.461	2235	2242	2248	rVB4	8831	17403	1.01%	0.190%
12	16.901	2311	2317	2325	rBV4	17083	39168	2.28%	0.428%
13	17.518	2415	2422	2433	rBV	376654	599129	34.81%	6.546%
14	18.676	2614	2619	2626	rBV	41036	83741	4.87%	0.915%
15	20.115	2858	2864	2871	rBV	1293268	1721032	100.00%	18.805%
16	20.897	2993	2997	3000	rBV	16570	19674	1.14%	0.215%
17	21.414	3081	3085	3102	rBV2	38305	100366	5.83%	1.097%
18	21.813	3146	3153	3166	rBV	377299	659424	38.32%	7.205%
19	21.972	3176	3180	3185	rVB	22091	32482	1.89%	0.355%
20	22.548	3274	3278	3283	rBV2	19944	36169	2.10%	0.395%
21	22.601	3283	3287	3292	rVB2	20515	33366	1.94%	0.365%
22	23.323	3406	3410	3419	rVB3	14747	30574	1.78%	0.334%
23	24.169	3549	3554	3560	rVB5	11129	23921	1.39%	0.261%
24	25.186	3716	3727	3738	rBV2	227746	695818	40.43%	7.603%

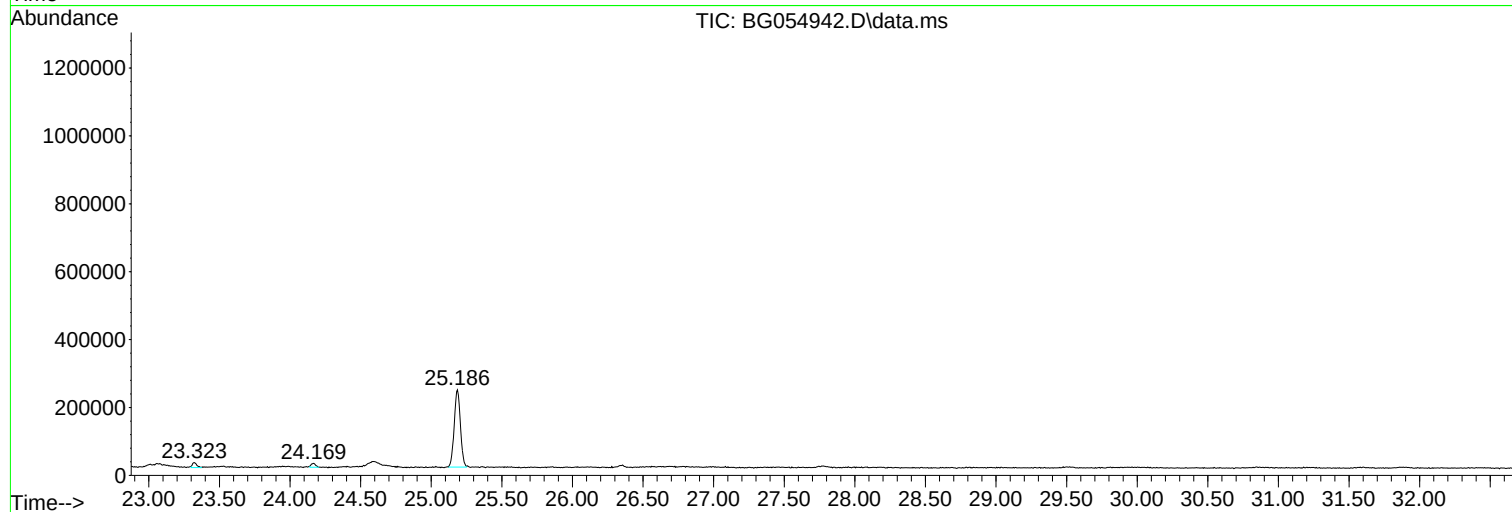
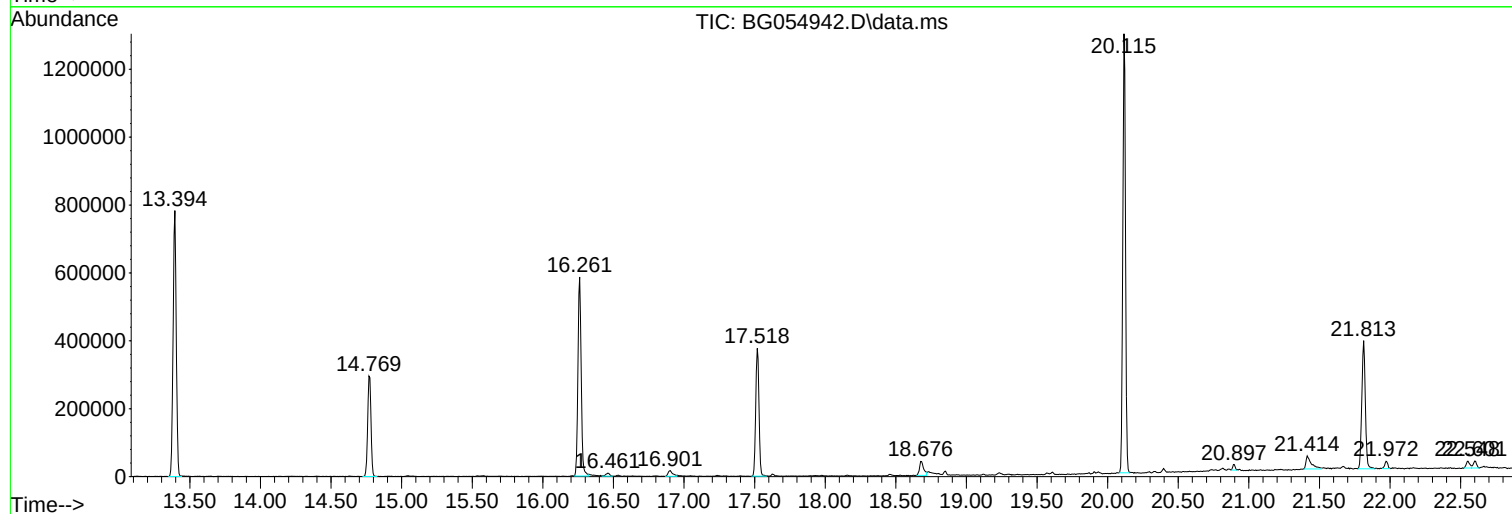
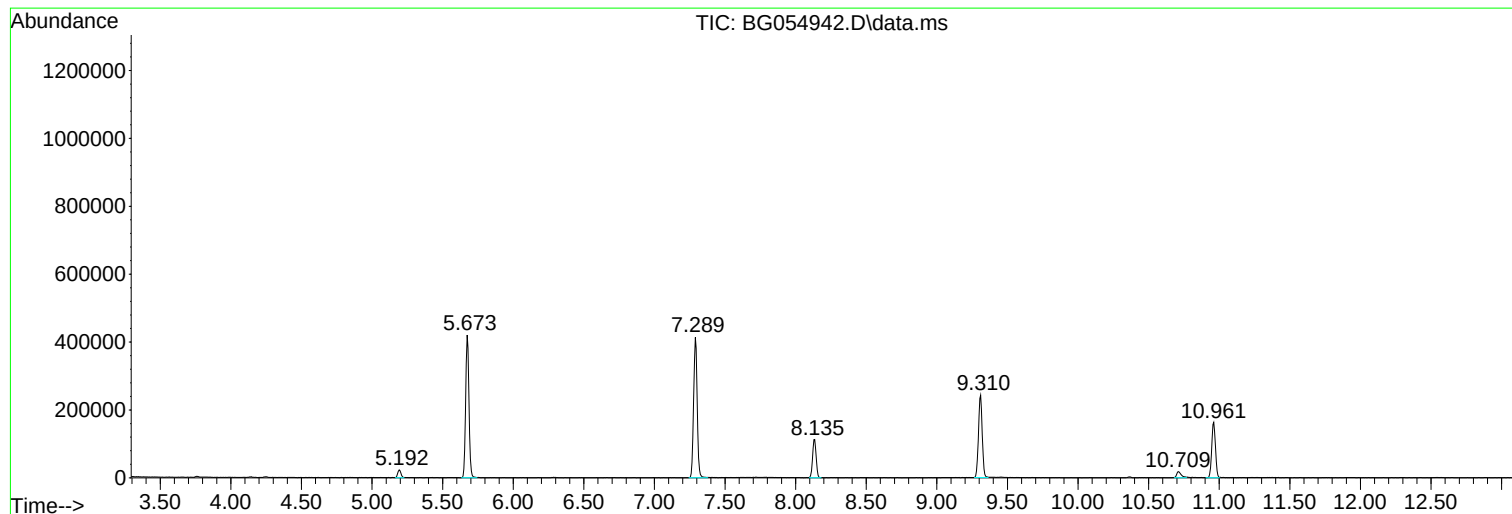
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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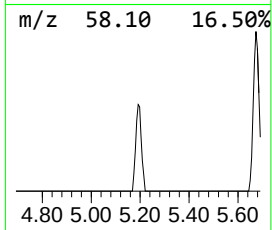
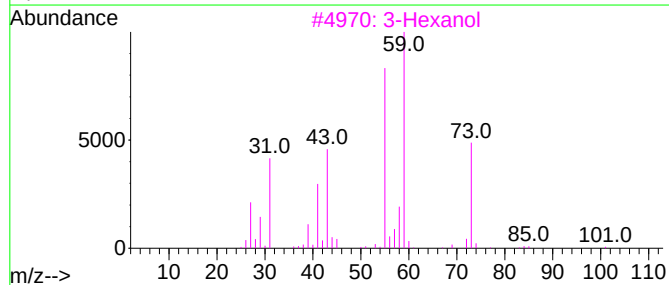
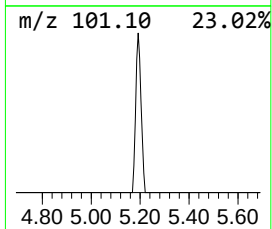
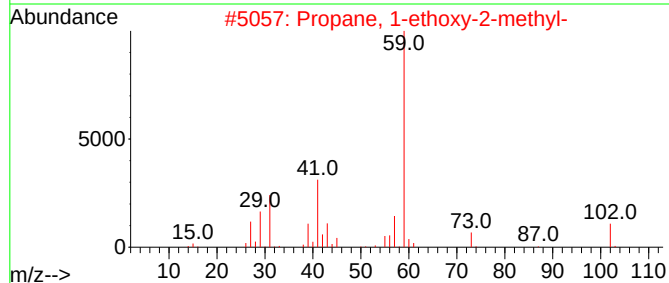
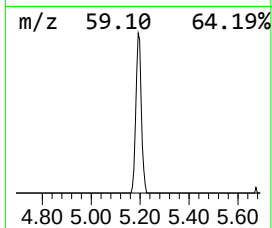
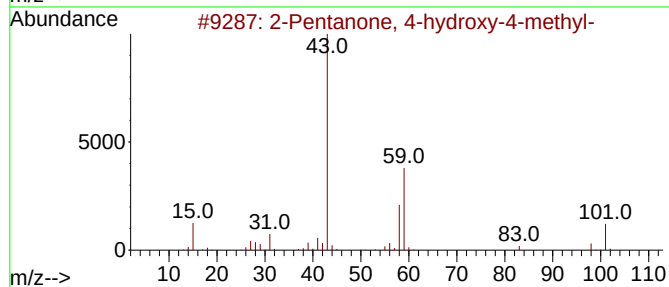
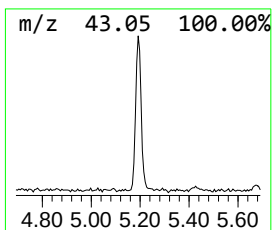
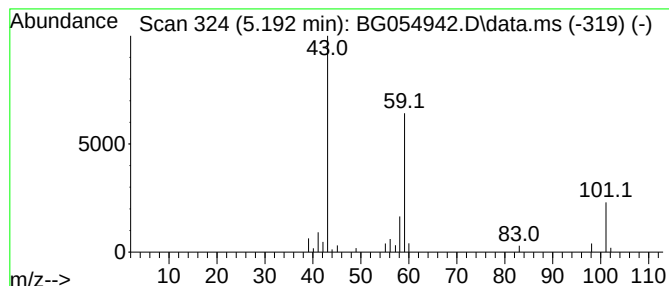
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.192	3.66 ng	36044	1,4-Dichlorobenzene-d4			8.129
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-		102	C6H14O	000627-02-1	38
3	3-Hexanol		102	C6H14O	000623-37-0	25
4	1-Butanol, 3-methoxy-		104	C5H12O2	002517-43-3	25
5	1,2-Butanediol		90	C4H10O2	000584-03-2	23



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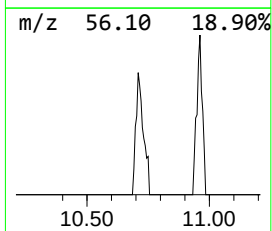
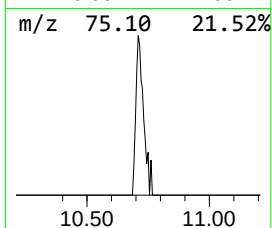
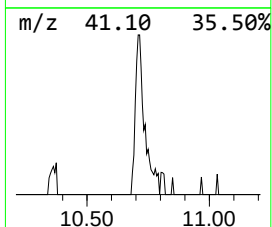
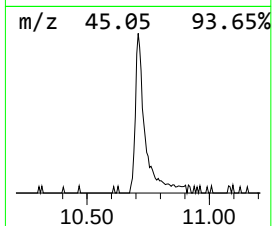
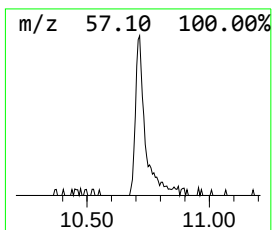
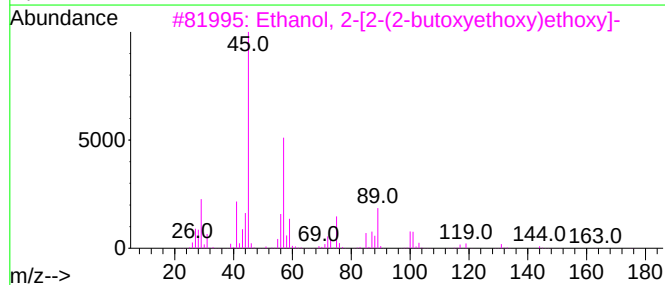
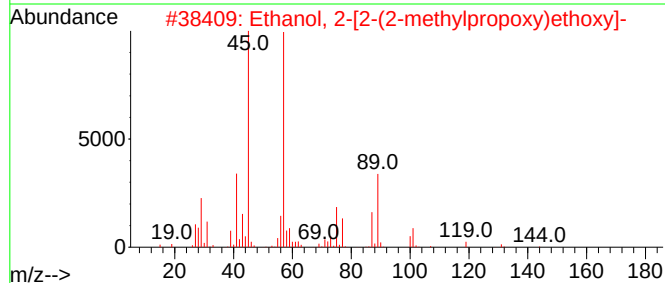
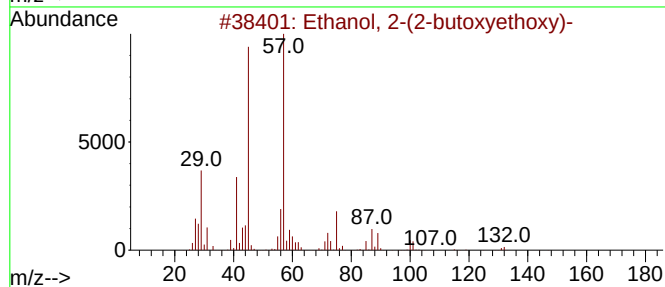
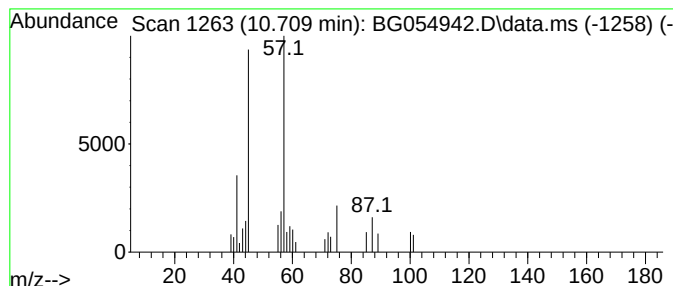
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.709	2.64 ng	39608	Naphthalene-d8	10.961	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
4	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	38
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	37



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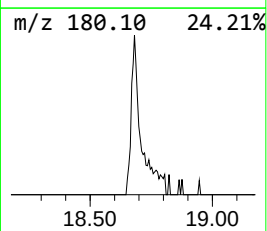
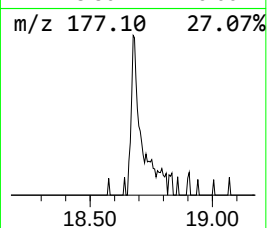
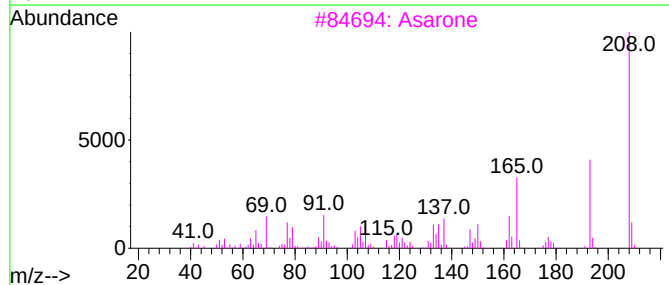
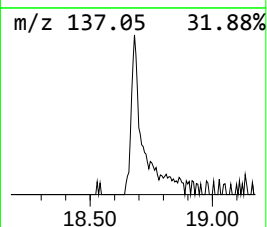
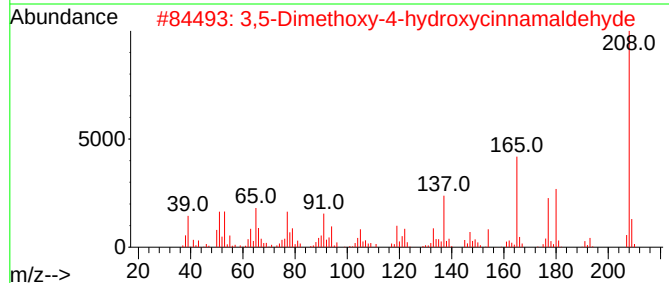
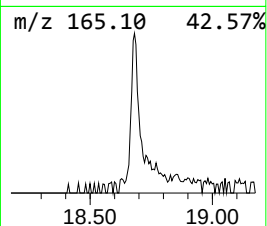
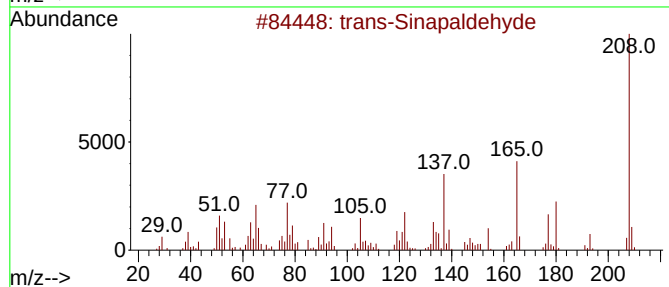
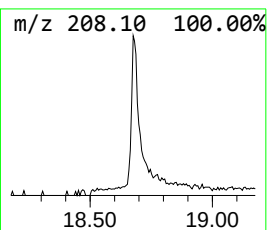
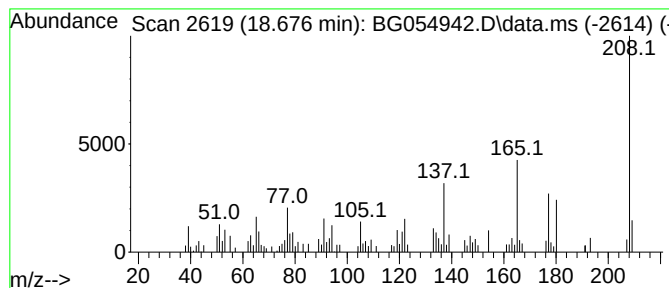
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Peak Number 3 trans-Sinapaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.676	2.80 ng	83741	Phenanthrene-d10	17.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapaldehyde	208	C11H12O4	004206-58-0	98
2			3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	C11H12O4	087345-53-7	98
3			Asarone	208	C12H16O3	002883-98-9	58
4			2H-1-Benzopyran-2-one, 7,8-dihydro	208	C10H8O5	000574-84-5	58
5			Benzenamide, N-cyano-3,4,5-trimethoxy	208	C10H12N2O3	055305-77-6	53



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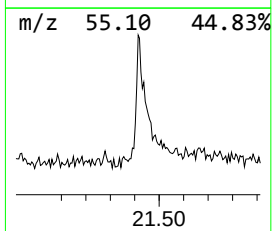
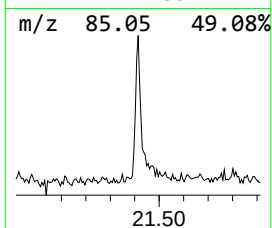
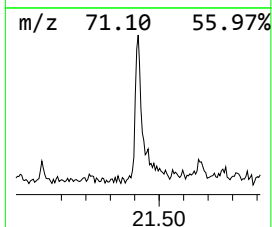
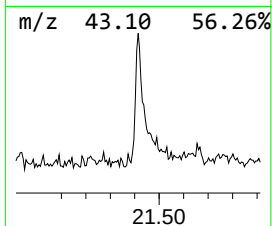
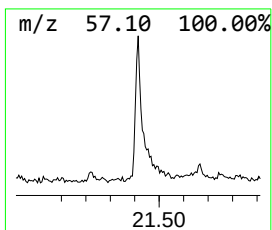
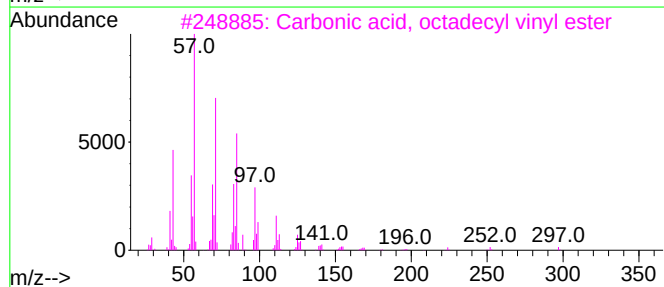
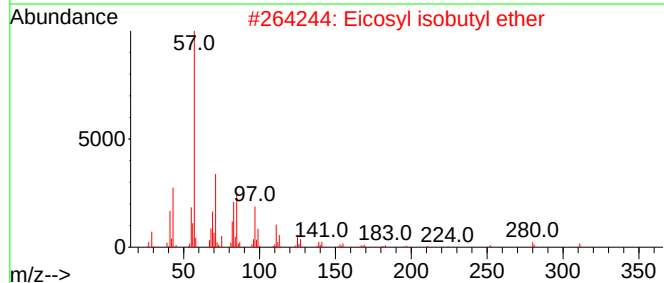
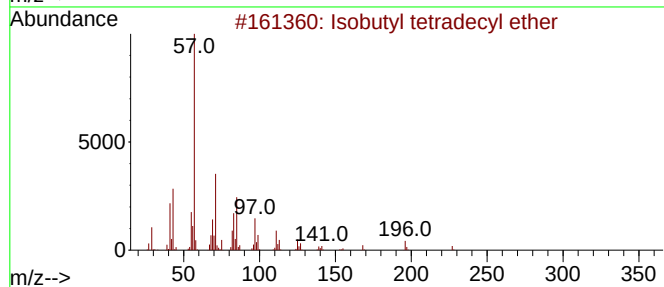
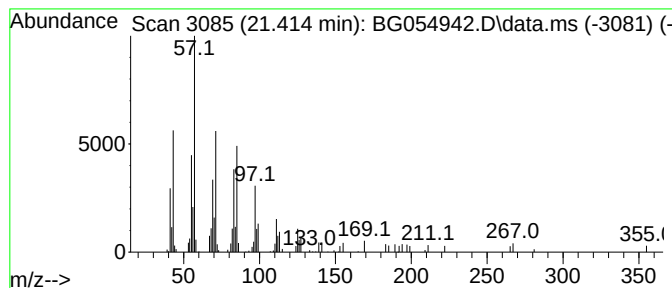
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Isobutyl tetradecyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.414	3.04 ng	100366	Chrysene-d12	21.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl tetradecyl ether	270	C18H38O	1000406-32-7	91
2			Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	91
3			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	87
4			Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	87
5			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.192	3.7	ng	36044	1	8.129	196901	20.0
Ethanol, 2-(2-b...	10.709	2.6	ng	39608	2	10.961	299550	20.0
trans-Sinapalde...	18.676	2.8	ng	83741	4	17.518	599129	20.0
Isobutyl tetrad...	21.414	3.0	ng	100366	5	21.813	659424	20.0