

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101220\
 Data File : BG046846.D
 Acq On : 12 Oct 2020 14:22
 Operator : CG/JU
 Sample : L4291-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PAV-B4-100620-0-10

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-BG092220.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.570	31	39	45	rBV	56809	82191	2.86%	0.559%
2	4.715	228	234	239	rBV2	21823	32510	1.13%	0.221%
3	5.203	313	317	324	rVB	43681	68512	2.38%	0.466%
4	5.667	388	396	406	rBV	450531	710997	24.75%	4.832%
5	7.253	659	666	675	rVB	389213	668545	23.27%	4.544%
6	8.105	804	811	819	rVB	285889	485986	16.92%	3.303%
7	9.263	1000	1008	1017	rVB	309387	559337	19.47%	3.801%
8	10.914	1280	1289	1299	rBV	340339	621688	21.64%	4.225%
9	13.352	1697	1704	1710	rBV	769052	1180121	41.08%	8.021%
10	14.169	1838	1843	1849	rBV2	26501	37819	1.32%	0.257%
11	14.727	1932	1938	1949	rVB	557986	864451	30.09%	5.875%
12	16.208	2183	2190	2203	rBV	753595	1154535	40.19%	7.847%
13	17.471	2398	2405	2414	rVB	791212	1198470	41.72%	8.145%
14	18.346	2549	2554	2559	rBV2	74803	125729	4.38%	0.855%
15	19.615	2766	2770	2775	rBV8	30619	49100	1.71%	0.334%
16	19.762	2791	2795	2800	rVB	169982	199124	6.93%	1.353%
17	19.880	2812	2815	2821	rVB5	27342	35324	1.23%	0.240%
18	20.074	2842	2848	2856	rVB	2181737	2872879	100.00%	19.525%
19	20.802	2968	2972	2978	rVB	129058	144569	5.03%	0.983%
20	21.378	3066	3070	3080	rVB3	68136	122340	4.26%	0.831%
21	21.625	3108	3112	3116	rBV5	22549	33169	1.15%	0.225%
22	21.742	3125	3132	3139	rVB	1006904	1696810	59.06%	11.532%
23	21.942	3161	3166	3170	rBV3	25841	39130	1.36%	0.266%
24	23.264	3387	3391	3397	rVB5	27511	48137	1.68%	0.327%
25	25.009	3676	3688	3701	rBV3	561264	1682117	58.55%	11.432%

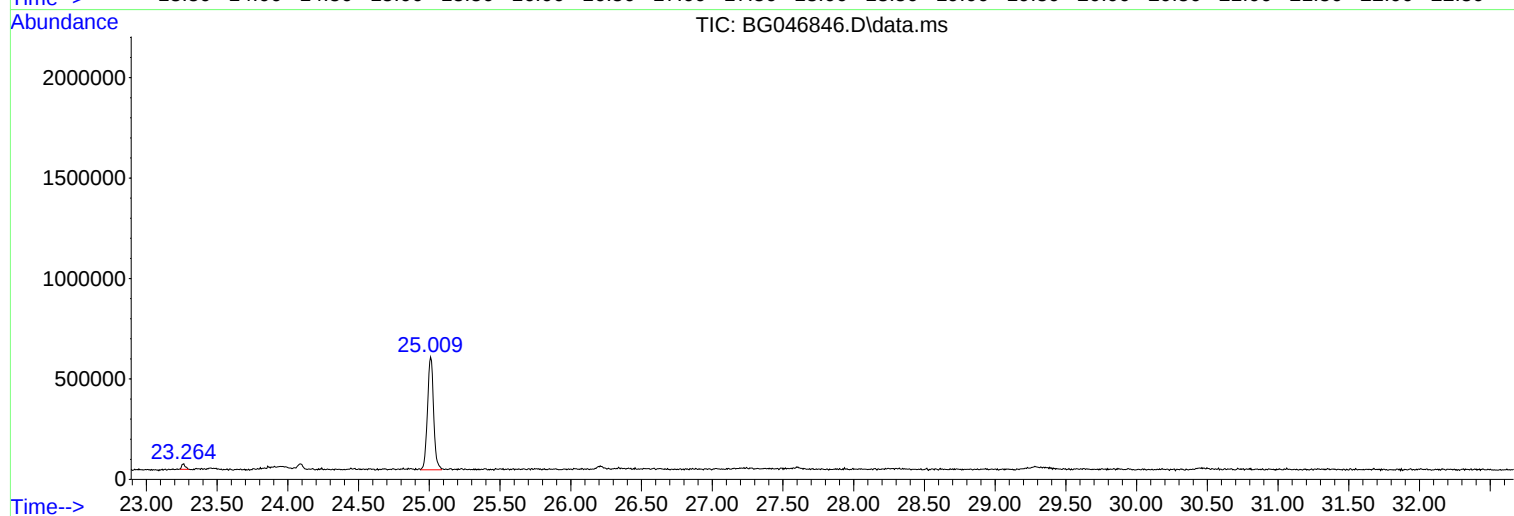
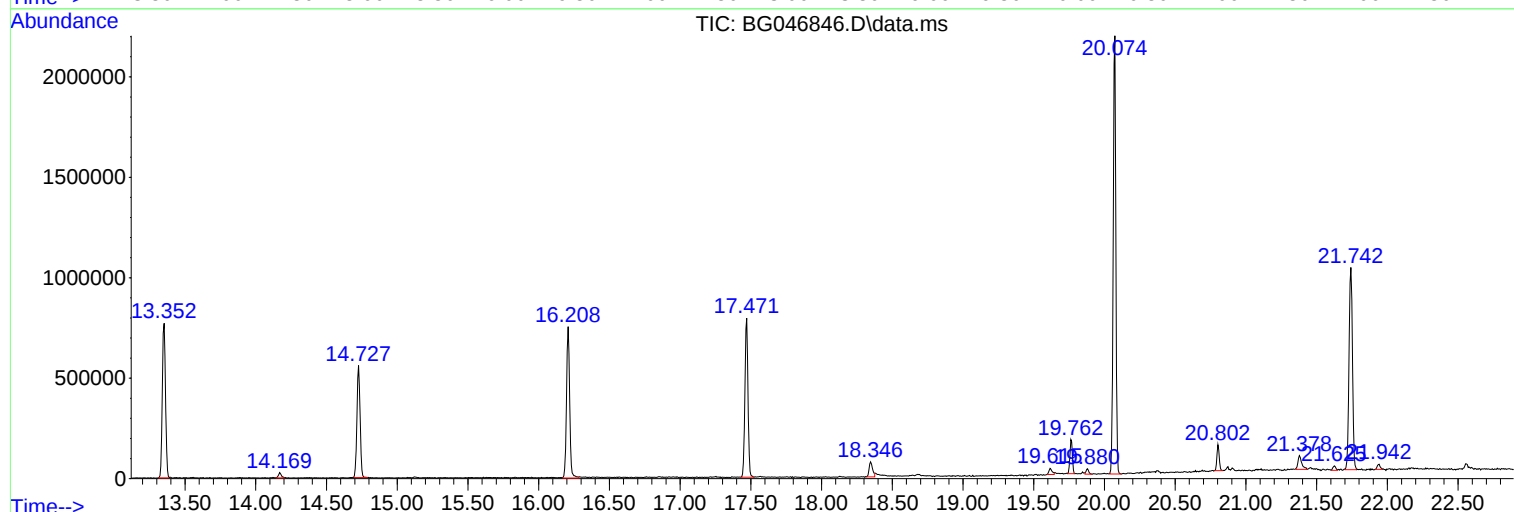
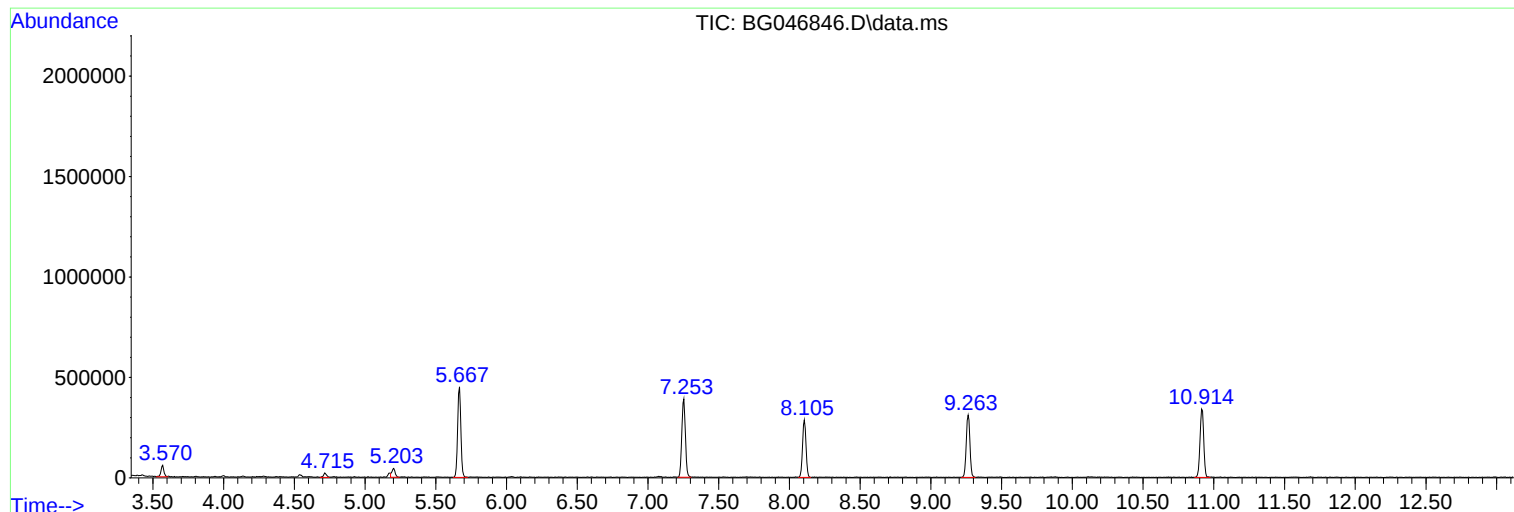
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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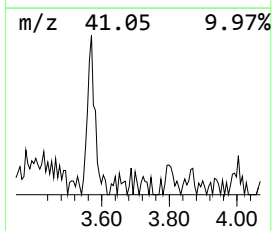
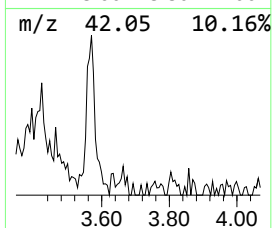
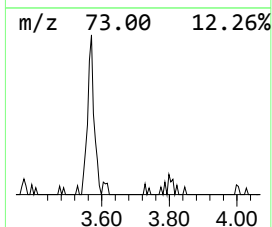
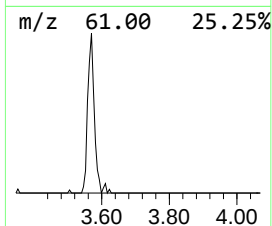
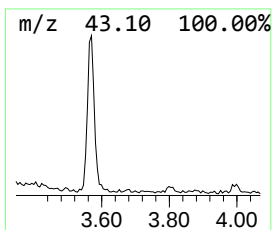
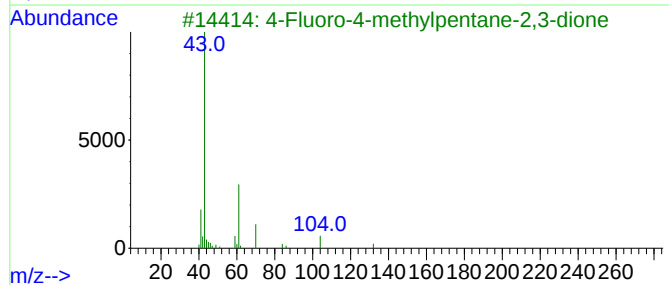
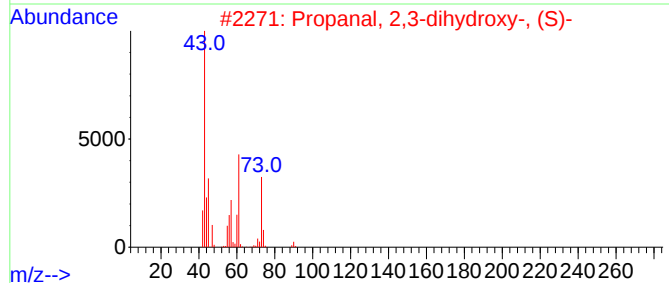
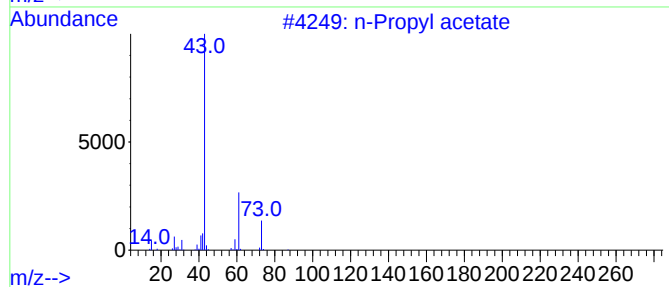
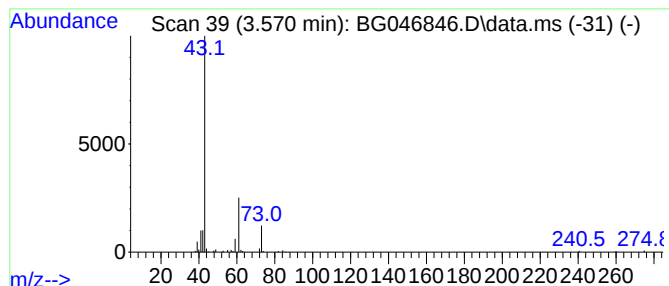
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.570	3.38 ng	82191	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	64
2			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
3			4-Fluoro-4-methylpentane-2,3-dione	132	C6H9F02	1000367-34-8	9
4			1-Propanol, 3-chloro-, acetate	136	C5H9ClO2	000628-09-1	9
5			1-Pentanol, 5-chloro-, acetate	164	C7H13ClO2	020395-28-2	9



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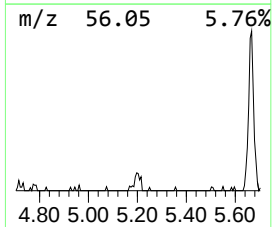
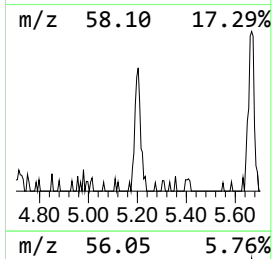
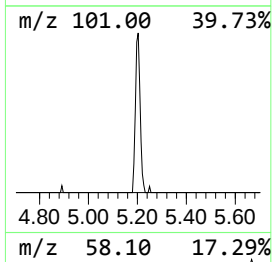
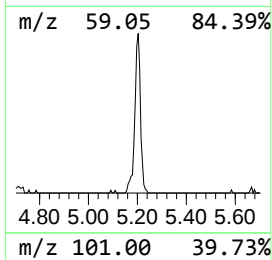
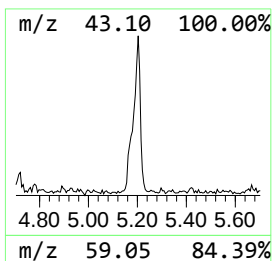
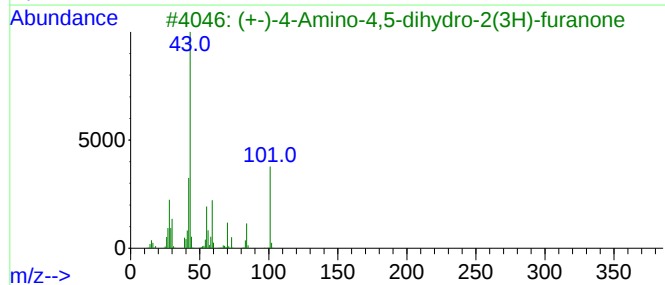
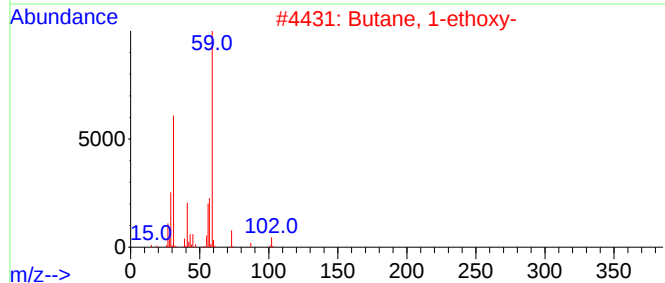
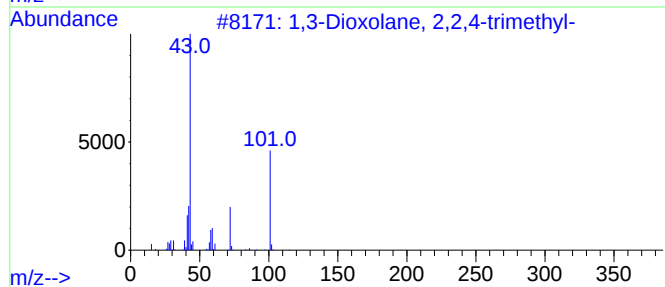
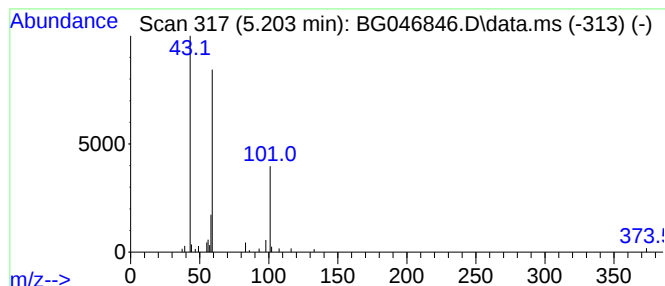
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Peak Number 2 unknown5.20 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.203	2.82 ng	68512	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	25
2			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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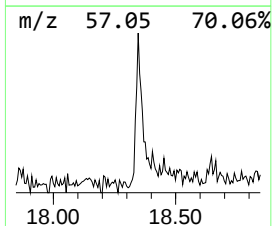
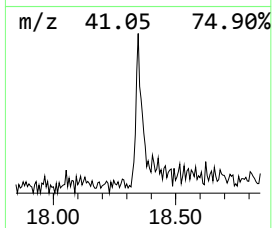
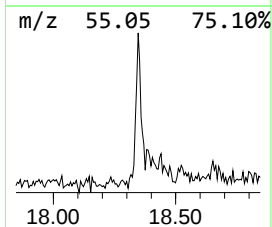
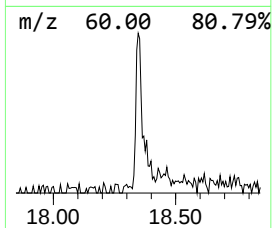
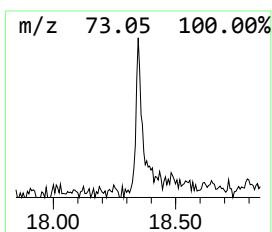
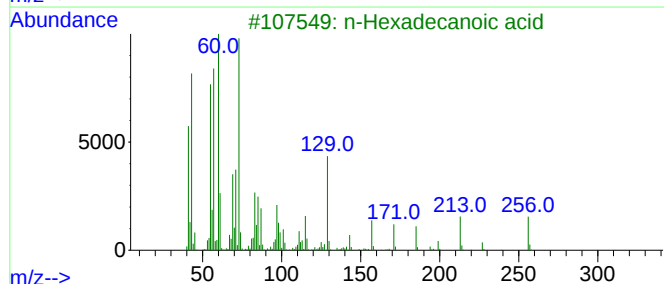
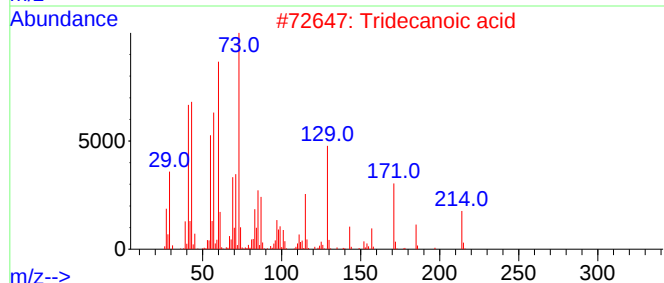
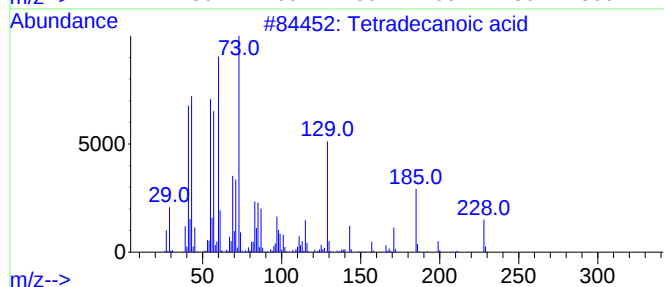
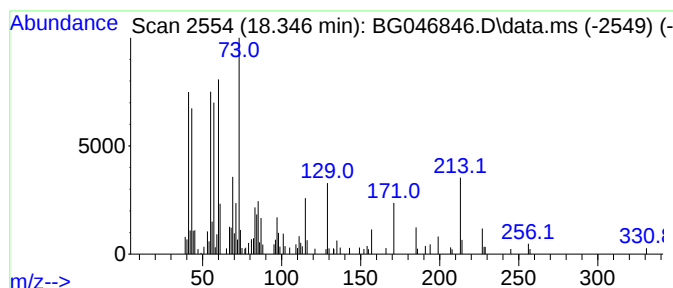
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Peak Number 3 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.346	2.10 ng	125729	Phenanthrene-d10	17.471

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
5			Octadecanoic acid	284	C18H36O2	000057-11-4	52



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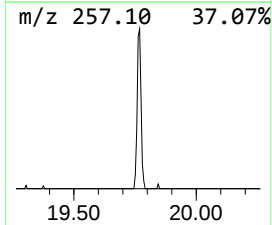
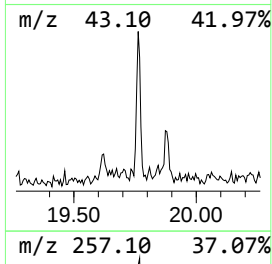
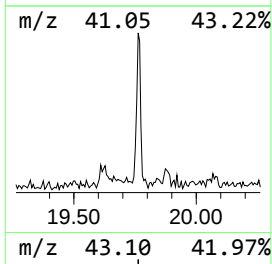
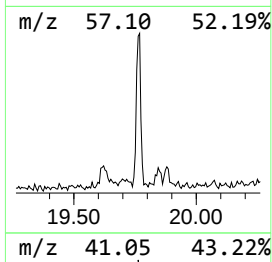
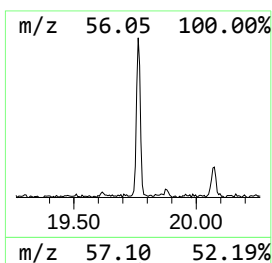
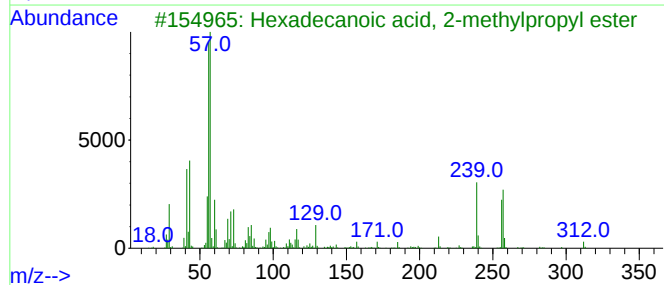
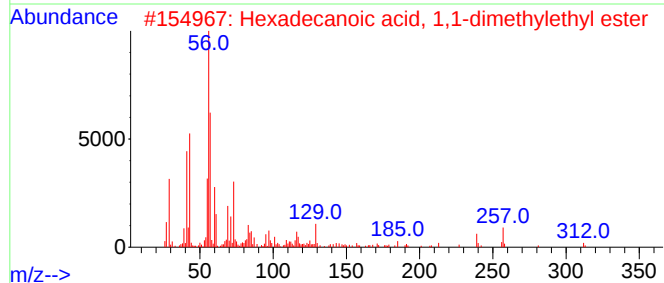
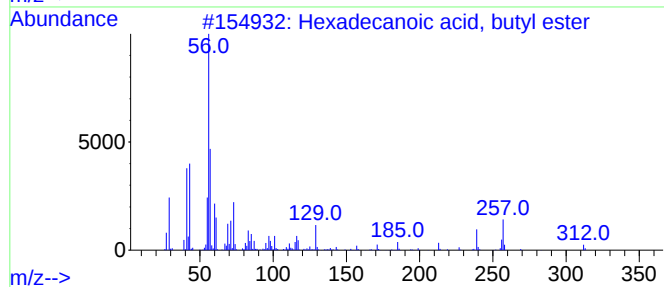
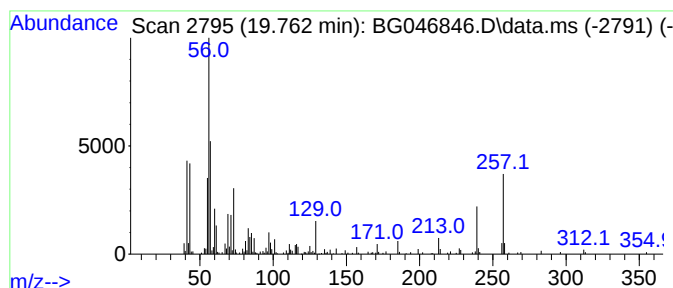
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.762	2.35 ng	199124	Chrysene-d12	21.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	52
4			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	38
5			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	3.570	3.4	ng	82191	1	8.105	485986	20.0
unknown5.20	5.203	2.8	ng	68512	1	8.105	485986	20.0
Tetradecanoic acid	18.346	2.1	ng	125729	4	17.471	1198470	20.0
Hexadecanoic ac...	19.762	2.4	ng	199124	5	21.742	1696810	20.0