

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102918\
 Data File : BG037628.D
 Acq On : 29 Oct 2018 18:30
 Operator : JU/SJ
 Sample : J5691-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-8

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG101818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.765	77	81	87	rBV	28443	43055	1.24%	0.204%
2	5.181	316	322	331	rBV	46333	76983	2.22%	0.365%
3	5.645	390	401	411	rBV	964021	1625843	46.97%	7.700%
4	7.249	663	674	690	rBV	1044944	1956609	56.53%	9.266%
5	7.625	729	738	750	rBV	955943	1720053	49.69%	8.146%
6	8.101	812	819	829	rBV	183914	324933	9.39%	1.539%
7	8.424	866	874	882	rVB	688081	1224176	35.37%	5.798%
8	9.276	1011	1019	1028	rBV	600419	1125703	32.52%	5.331%
9	10.921	1292	1299	1309	rBV	277838	503020	14.53%	2.382%
10	13.353	1705	1713	1727	rBV	1524180	2508940	72.48%	11.882%
11	14.176	1846	1853	1864	rBV	210325	331134	9.57%	1.568%
12	14.734	1941	1948	1958	rVB2	468880	769535	22.23%	3.644%
13	16.221	2194	2201	2212	rBV	1306849	2045746	59.10%	9.689%
14	17.484	2409	2416	2425	rBV2	606351	967032	27.94%	4.580%
15	18.336	2556	2561	2569	rBV2	40994	69508	2.01%	0.329%
16	20.081	2852	2858	2867	rBV	2552156	3461426	100.00%	16.393%
17	21.368	3072	3077	3091	rBV3	57521	132984	3.84%	0.630%
18	21.761	3138	3144	3157	rBV2	563123	1006328	29.07%	4.766%
19	21.920	3167	3171	3178	rVB2	28822	43415	1.25%	0.206%
20	22.543	3272	3277	3283	rBV2	26486	42425	1.23%	0.201%
21	23.254	3393	3398	3407	rVB3	26870	56452	1.63%	0.267%
22	24.082	3533	3539	3547	rBV4	25169	60738	1.75%	0.288%
23	25.099	3698	3712	3728	rBV2	284256	978011	28.25%	4.632%
24	26.238	3895	3906	3909	rBV9	12521	41136	1.19%	0.195%

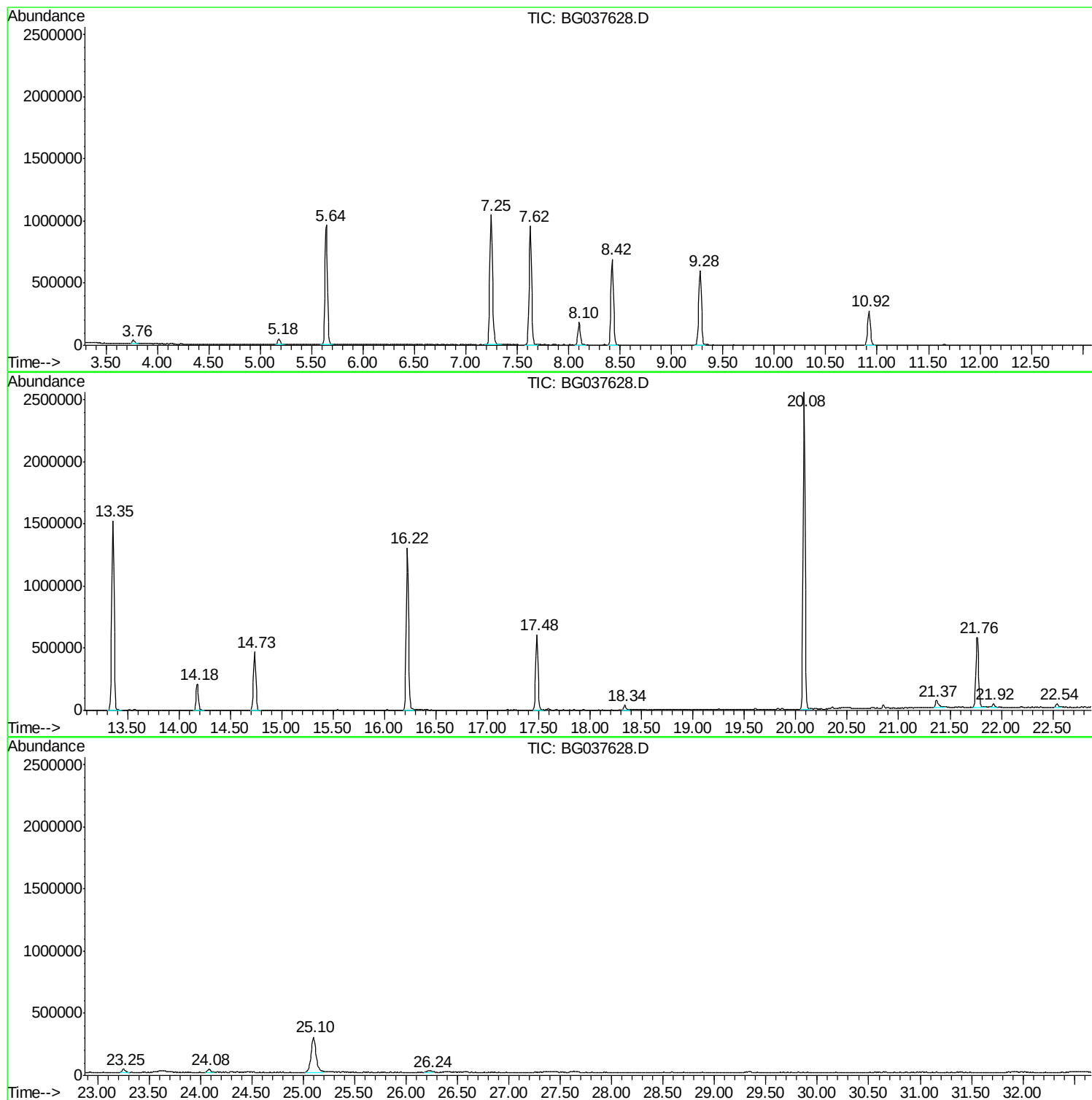
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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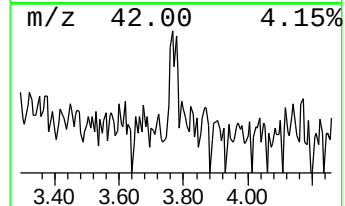
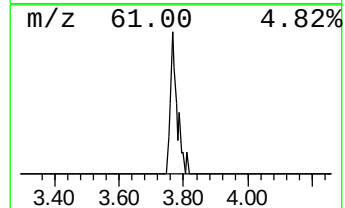
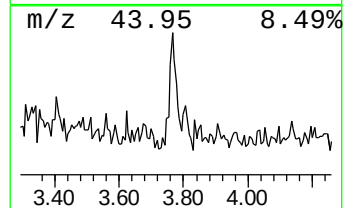
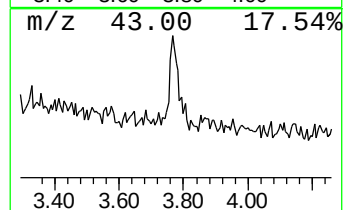
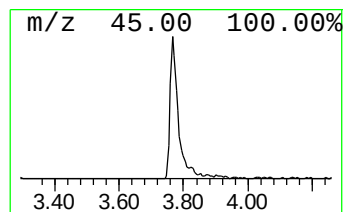
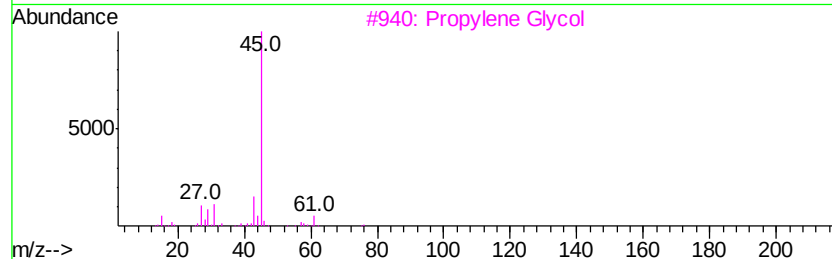
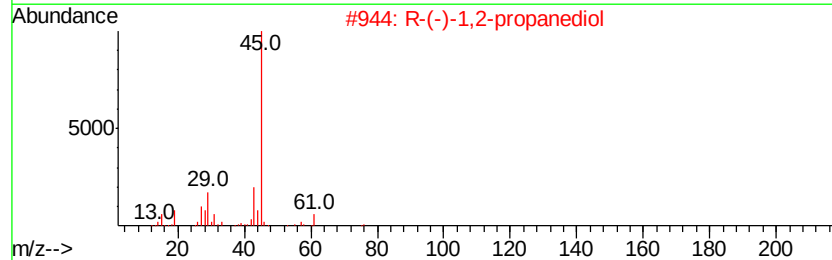
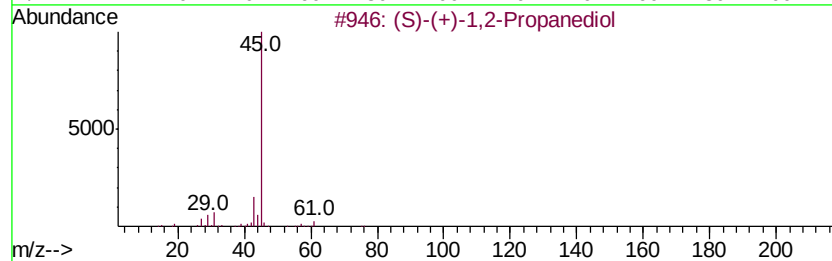
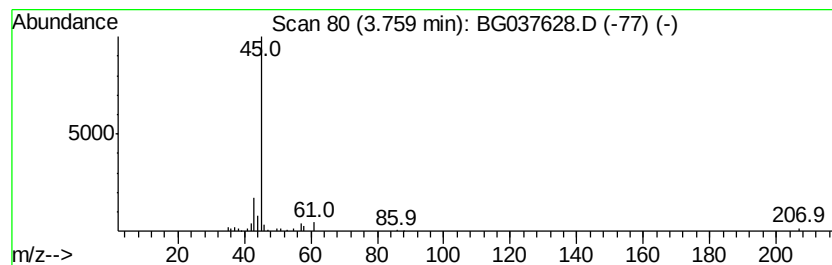
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	2.65 ng	43055	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5		Formamide	45	CH3NO	000075-12-7	7



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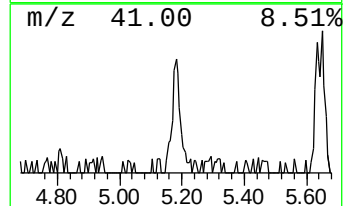
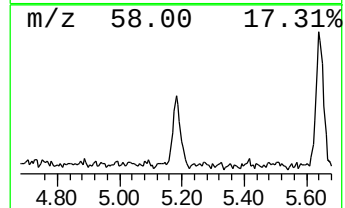
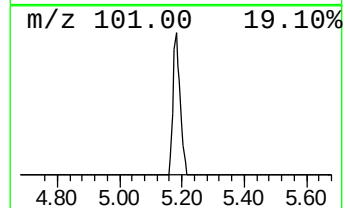
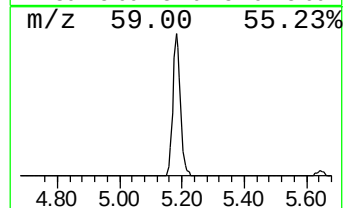
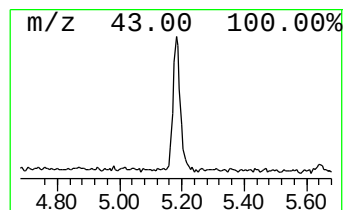
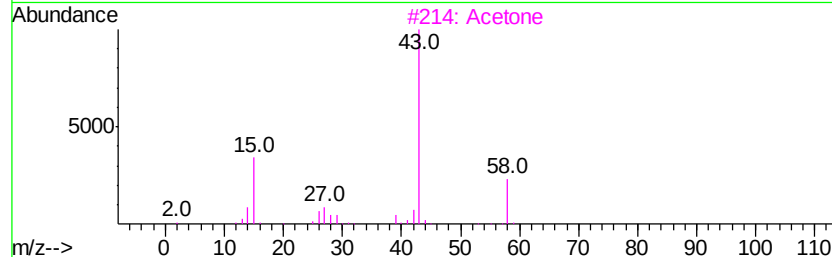
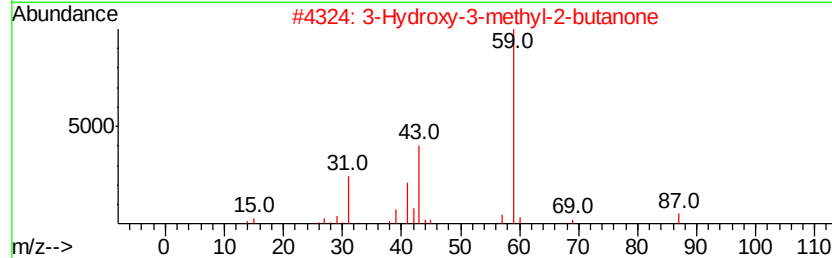
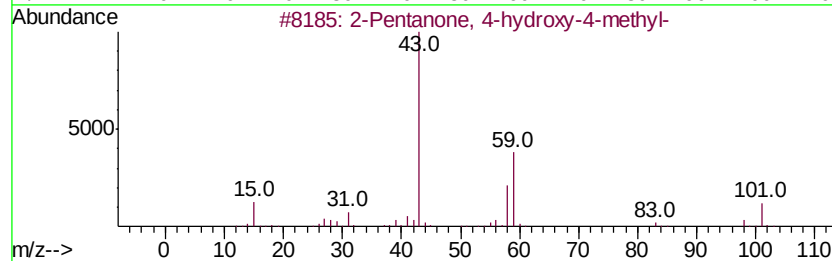
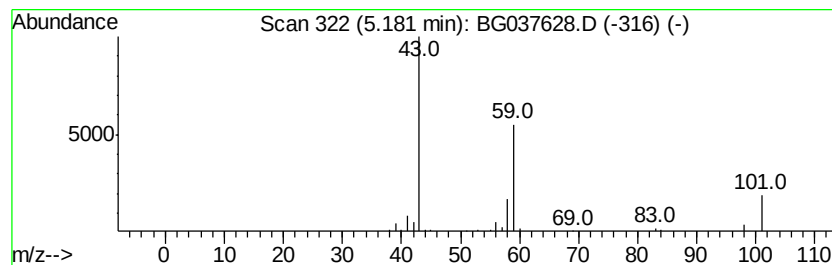
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	4.74 ng	76983	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
2		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
3		Acetone	58	C3H6O	000067-64-1	10
4		3-Octanol	130	C8H18O	000589-98-0	9
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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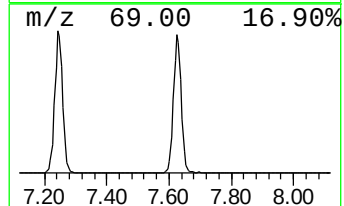
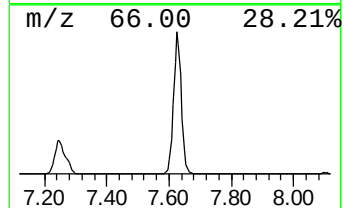
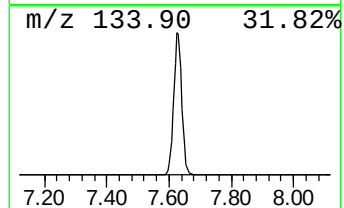
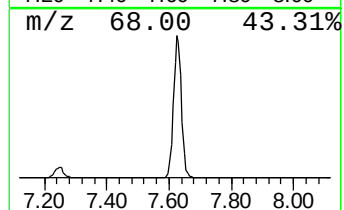
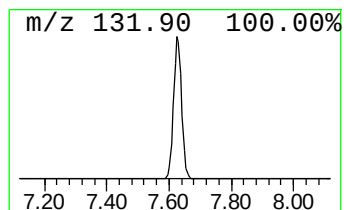
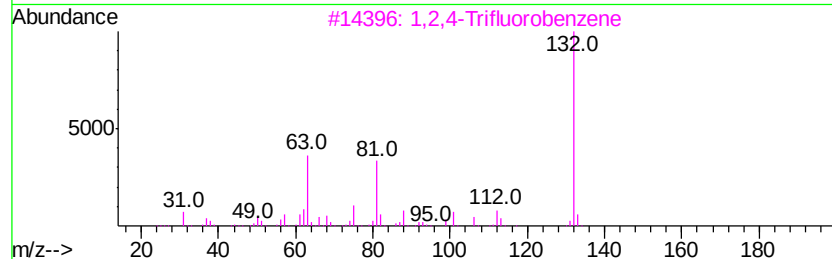
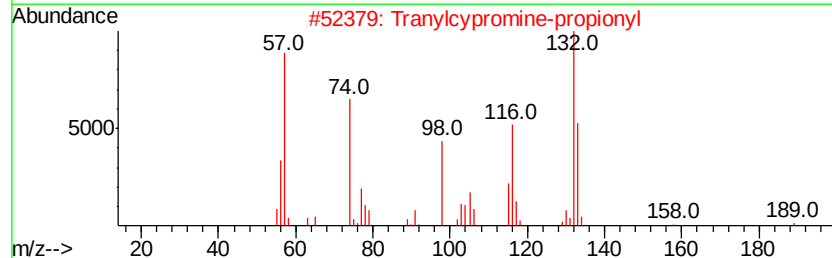
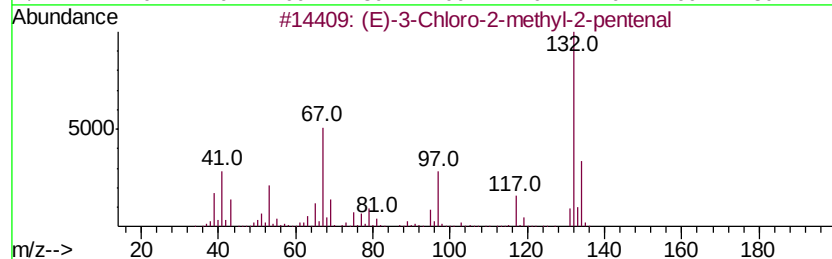
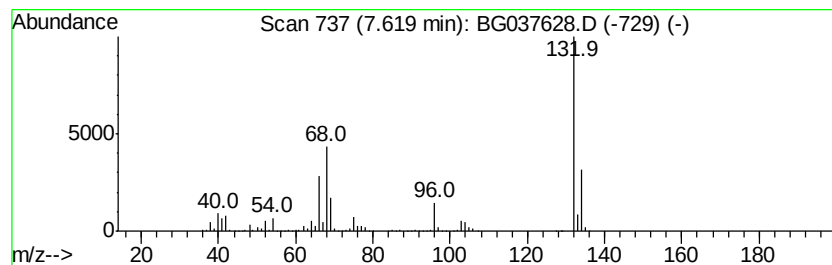
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Peak Number 3 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	105.87 ng	1720050	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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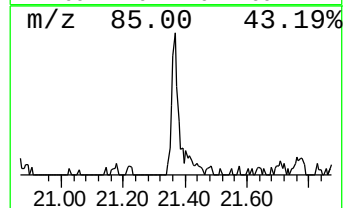
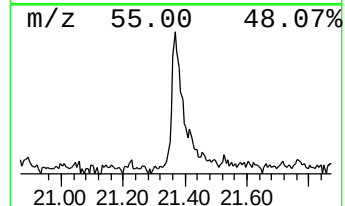
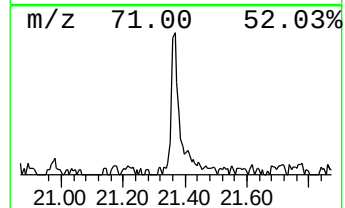
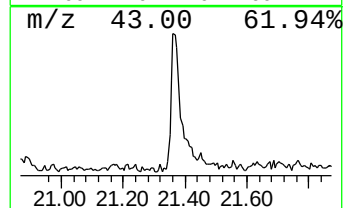
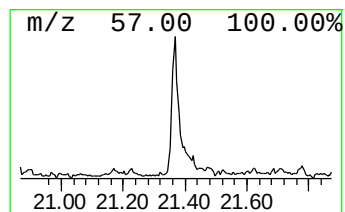
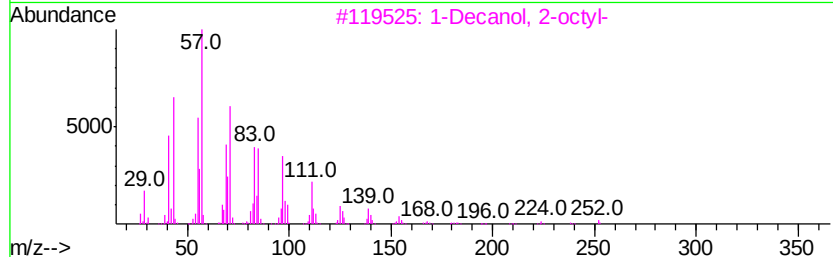
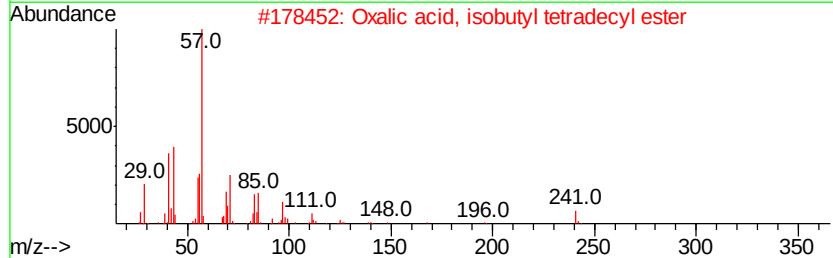
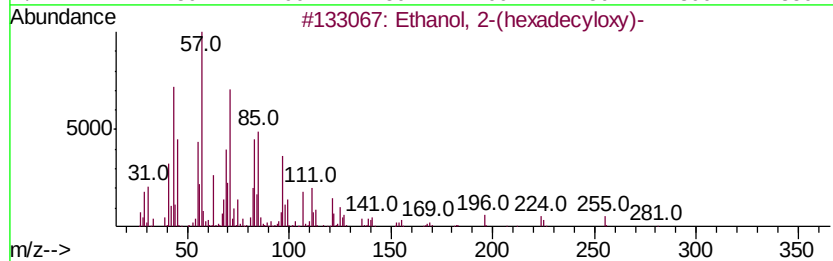
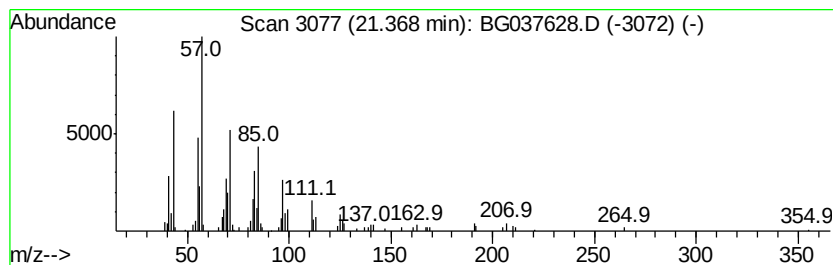
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Peak Number 5 Ethanol, 2-(hexadecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	2.64 ng	132984	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	90
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
5		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.76	2.6	ng	43055	1	8.10	324933	20.0
2-Pentanone, 4-hy...	5.18	4.7	ng	76983	1	8.10	324933	20.0
unknown7.62	7.62	105.9	ng	1720050	1	8.10	324933	20.0
Ethanol, 2-(hexad...	21.37	2.6	ng	132984	5	21.76	1006330	20.0