

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102918\
Data File : BG037630.D
Acq On : 29 Oct 2018 19:48
Operator : JU/SJ
Sample : J5691-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-9

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-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	92	rBV	33823	55985	1.80%	0.285%
2	5.181	315	322	331	rBV	39924	71129	2.28%	0.362%
3	5.645	394	401	414	rVB	876199	1467153	47.06%	7.477%
4	7.243	665	673	689	rBV	933242	1780242	57.11%	9.073%
5	7.625	731	738	756	rVB	866995	1549077	49.69%	7.895%
6	8.101	812	819	830	rBV	193781	341556	10.96%	1.741%
7	8.424	867	874	883	rBV	627822	1113653	35.72%	5.675%
8	9.276	1011	1019	1030	rBV	540922	1005038	32.24%	5.122%
9	10.921	1292	1299	1308	rBV	285264	527268	16.91%	2.687%
10	13.353	1705	1713	1725	rBV	1391997	2305424	73.95%	11.749%
11	14.176	1846	1853	1860	rBV	207913	308320	9.89%	1.571%
12	14.734	1941	1948	1956	rBV2	488127	806082	25.86%	4.108%
13	16.221	2194	2201	2211	rBV	1143512	1795190	57.59%	9.149%
14	17.484	2409	2416	2423	rBV	635985	1004124	32.21%	5.117%
15	18.336	2555	2561	2565	rBV2	46744	65045	2.09%	0.331%
16	20.081	2852	2858	2869	rBV	2278256	3117454	100.00%	15.887%
17	21.367	3073	3077	3089	rBV3	50470	116585	3.74%	0.594%
18	21.767	3138	3145	3157	rBV2	584908	1044540	33.51%	5.323%
19	22.537	3272	3276	3281	rBV3	21293	35972	1.15%	0.183%
20	23.253	3392	3398	3404	rBV2	25097	48152	1.54%	0.245%
21	24.082	3533	3539	3548	rVB5	25384	56074	1.80%	0.286%
22	25.098	3700	3712	3730	rBV2	283104	963616	30.91%	4.911%
23	26.226	3898	3904	3912	rVB10	15721	44518	1.43%	0.227%

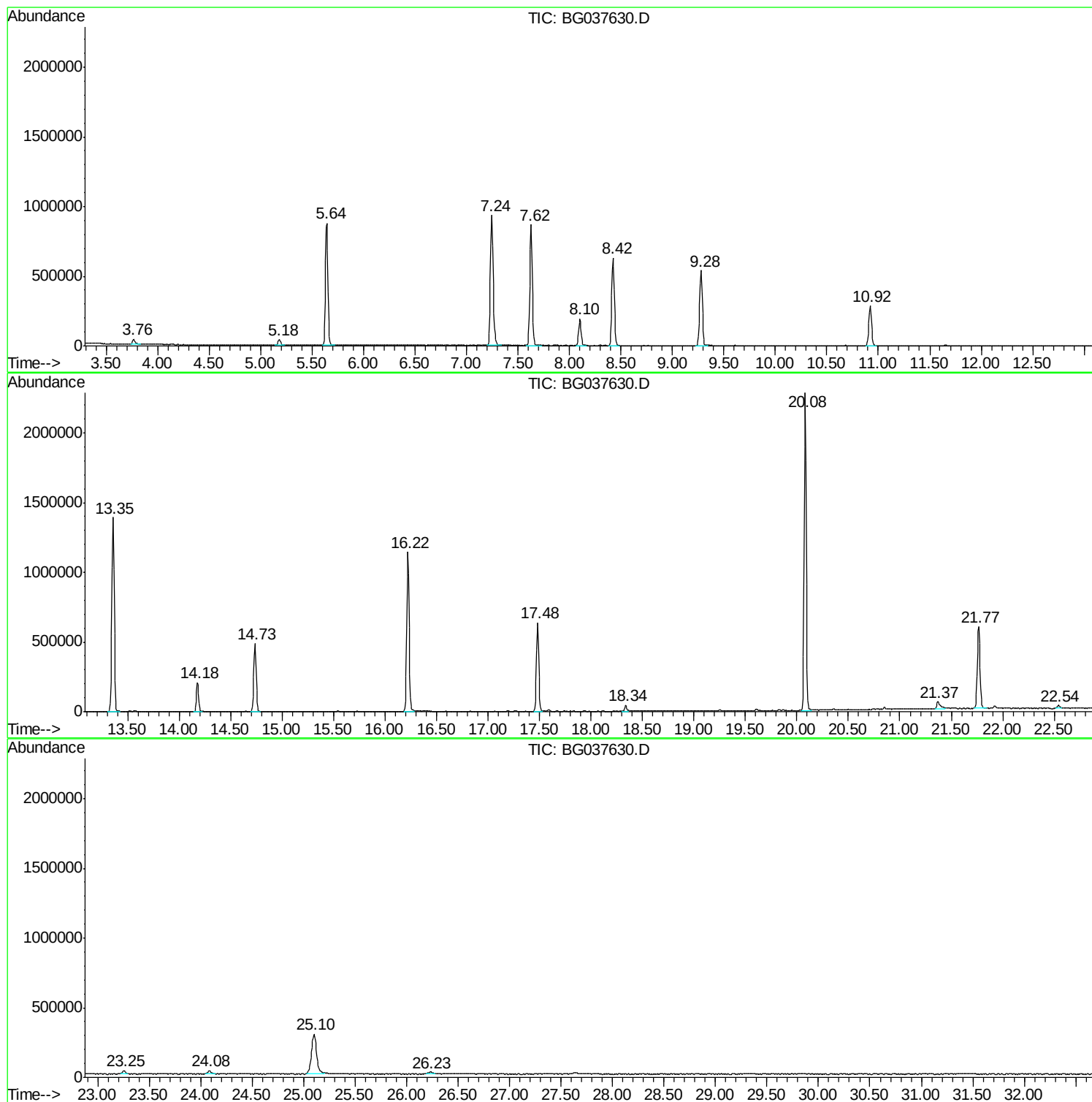
Sum of corrected areas: 19622197

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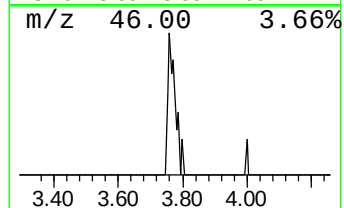
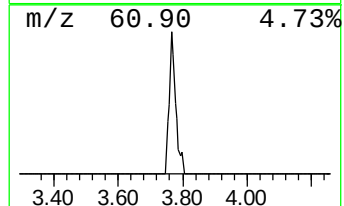
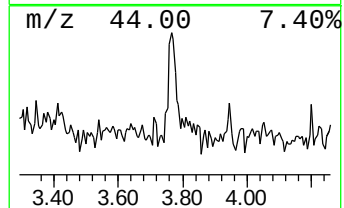
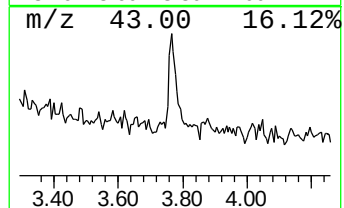
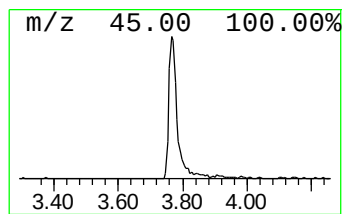
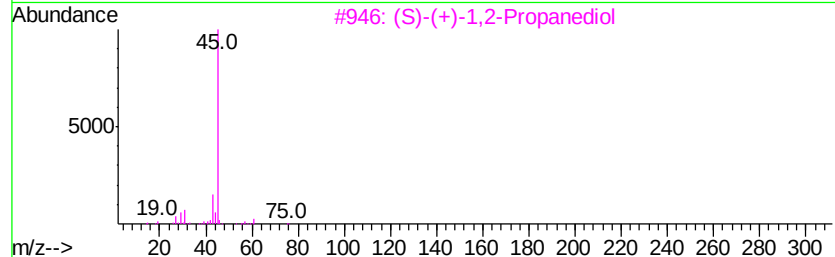
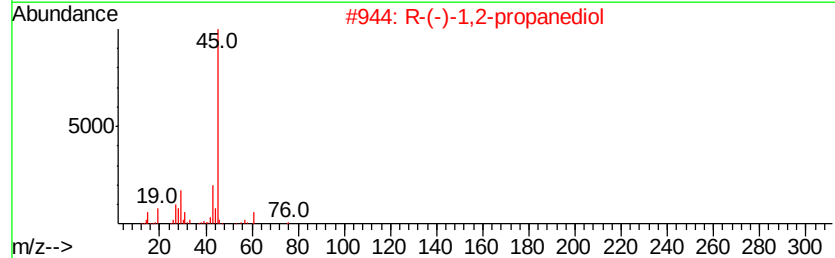
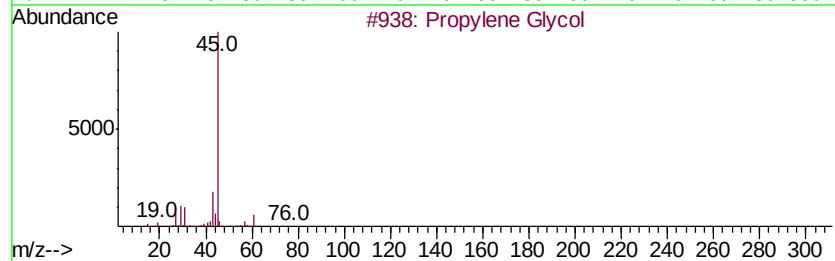
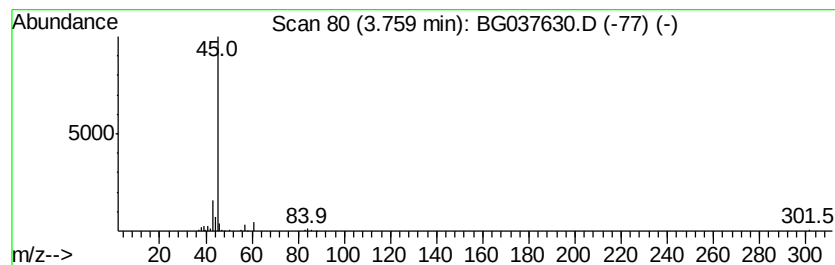
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	3.28 ng	55985	1,4-Dichlorobenzene-d4	8.10

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



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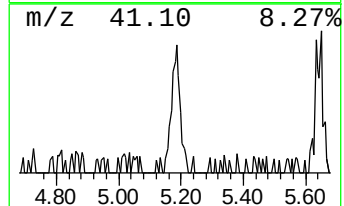
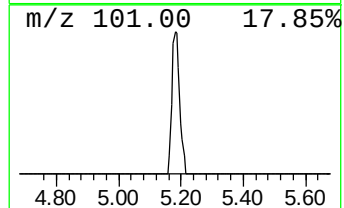
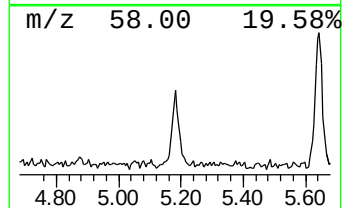
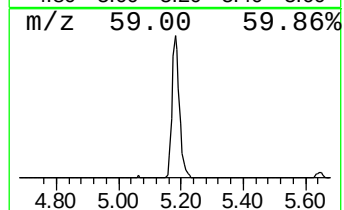
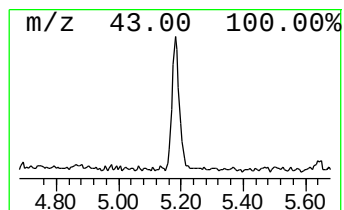
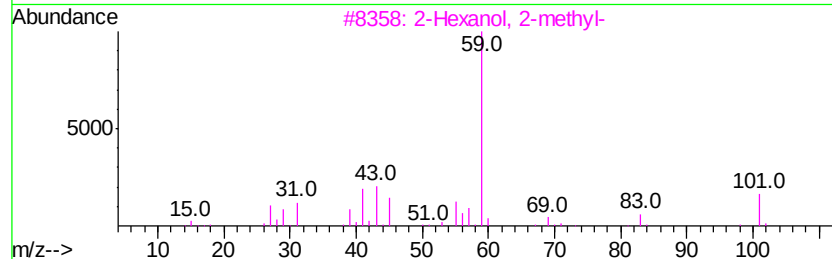
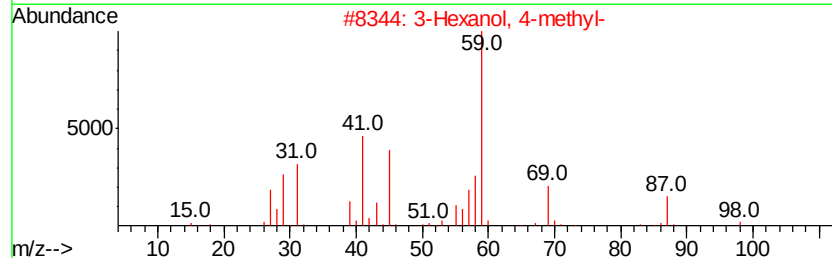
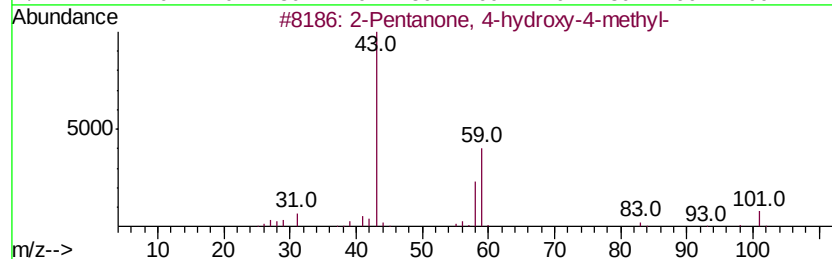
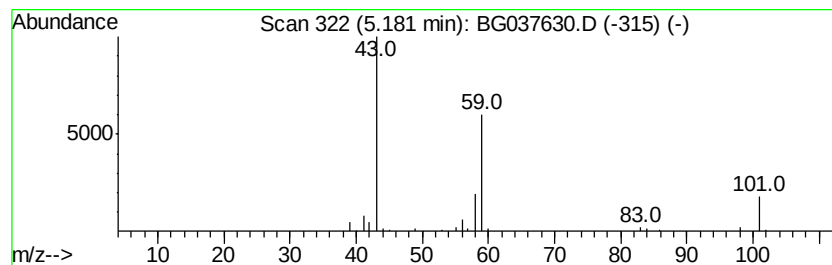
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	4.17 ng	71129	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	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	40
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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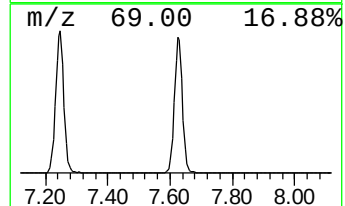
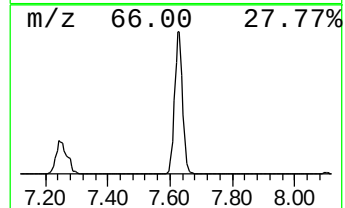
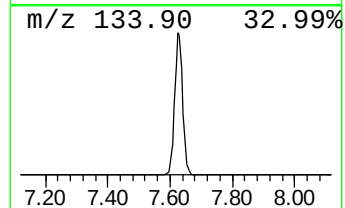
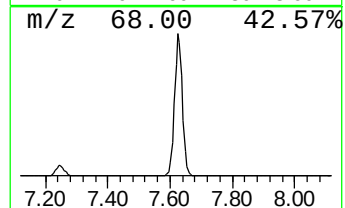
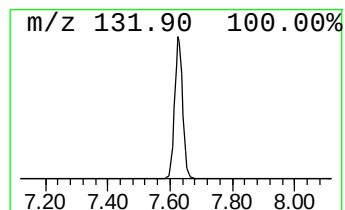
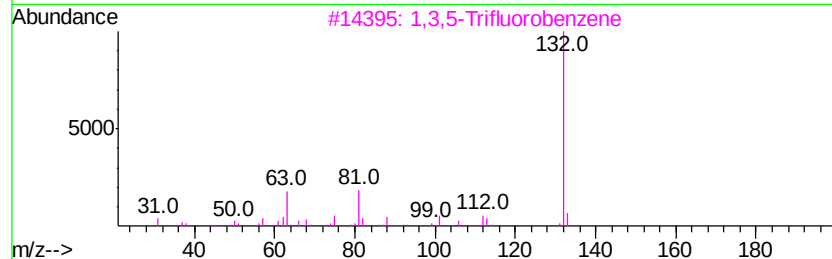
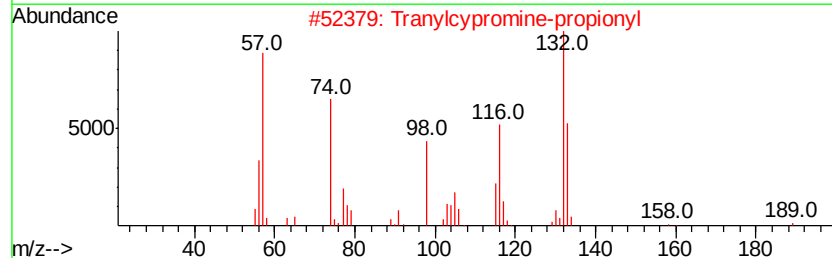
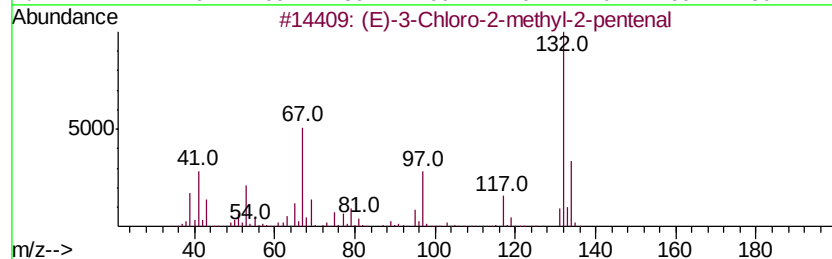
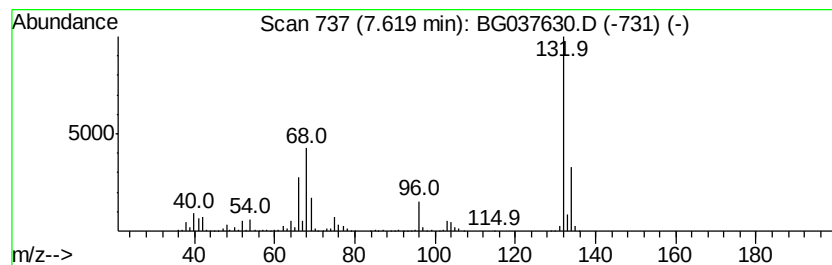
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Peak Number 3 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	90.71 ng	1549080	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	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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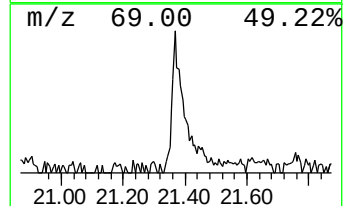
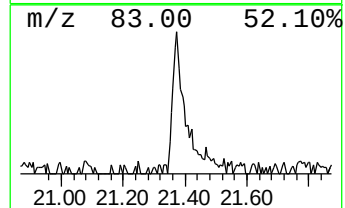
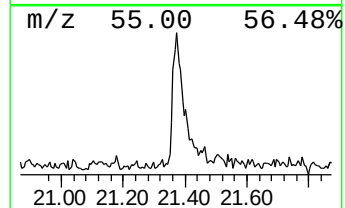
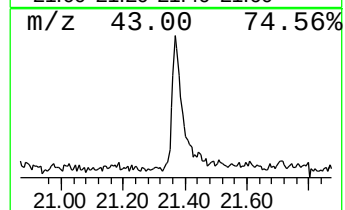
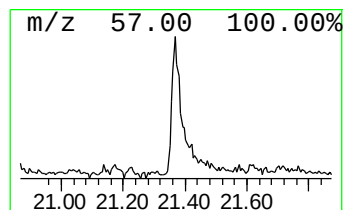
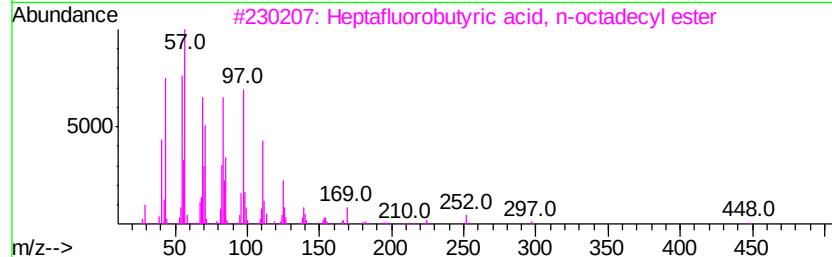
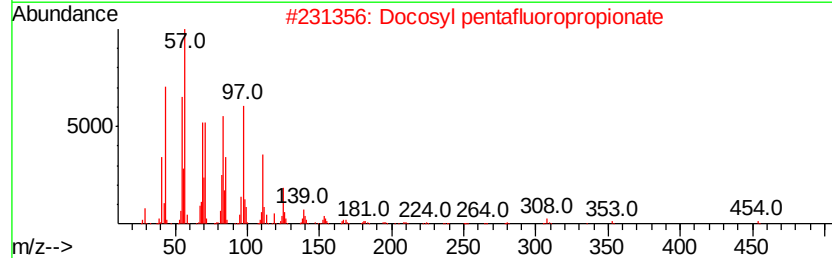
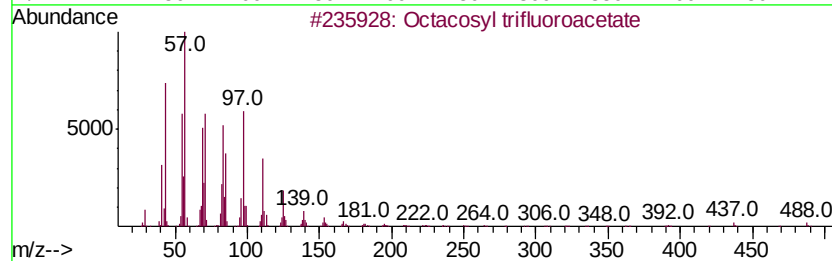
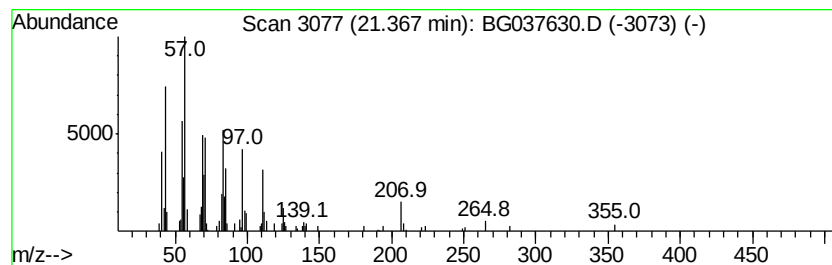
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Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	2.23 ng	116585	Chrysene-d12	21.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
2		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
3		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.76	3.3	ng	55985	1	8.10	341556	20.0
2-Pentanone, 4-hy...	5.18	4.2	ng	71129	1	8.10	341556	20.0
unknown7.62	7.62	90.7	ng	1549080	1	8.10	341556	20.0
Octacosyl trifluo...	21.37	2.2	ng	116585	5	21.77	1044540	20.0