

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010419\
 Data File : BG038927.D
 Acq On : 4 Jan 2019 12:39
 Operator : JU/SJ
 Sample : K1019-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TEST-PIT-D-11-12-A

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-BG121218.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	3.727	105	109	119	rBV	15924	28663	1.42%	0.240%
2	5.132	342	348	356	rVB	23749	38466	1.90%	0.322%
3	5.602	420	428	439	rBV	407875	704411	34.86%	5.900%
4	7.206	693	701	714	rBV	445557	851525	42.14%	7.132%
5	7.576	756	764	776	rBV	427701	760948	37.66%	6.374%
6	8.046	837	844	851	rVB	97268	169623	8.39%	1.421%
7	8.369	889	899	908	rBV	321821	570993	28.26%	4.783%
8	9.227	1036	1045	1056	rBV	258410	490474	24.27%	4.108%
9	10.866	1317	1324	1332	rBV	134454	245576	12.15%	2.057%
10	13.304	1729	1739	1749	rBV	820006	1280462	63.37%	10.725%
11	14.133	1874	1880	1887	rBV	86230	132044	6.53%	1.106%
12	14.685	1967	1974	1981	rBV3	241646	393899	19.49%	3.299%
13	16.177	2221	2228	2248	rBV2	710151	1114256	55.14%	9.333%
14	17.435	2434	2442	2446	rBV2	340748	531999	26.33%	4.456%
15	17.476	2446	2449	2457	rVV	88009	132617	6.56%	1.111%
16	17.570	2460	2465	2474	rVB2	21344	31587	1.56%	0.265%
17	18.304	2585	2590	2595	rBV	15337	26077	1.29%	0.218%
18	18.357	2595	2599	2605	rVB2	17329	25791	1.28%	0.216%
19	18.504	2618	2624	2634	rBV4	18679	49820	2.47%	0.417%
20	19.485	2785	2791	2798	rBV	155316	221172	10.95%	1.852%
21	19.814	2842	2847	2849	rBV2	22318	34364	1.70%	0.288%
22	19.850	2849	2853	2859	rVB	131905	190795	9.44%	1.598%
23	20.038	2879	2885	2893	rBV	1534620	2020621	100.00%	16.924%
24	20.167	2902	2907	2914	rVB4	9650	21028	1.04%	0.176%
25	20.331	2932	2935	2939	rVB	19395	31420	1.55%	0.263%
26	20.490	2957	2962	2967	rVB3	11865	20674	1.02%	0.173%
27	21.307	3094	3101	3109	rBV6	28119	72887	3.61%	0.610%
28	21.712	3161	3170	3175	rBV2	362416	701370	34.71%	5.875%
29	21.759	3175	3178	3186	rVV	50637	89467	4.43%	0.749%
30	21.853	3189	3194	3199	rBV2	14655	22724	1.12%	0.190%
31	22.458	3292	3297	3303	rVB4	20736	36670	1.81%	0.307%
32	23.157	3408	3416	3421	rBV3	18873	46603	2.31%	0.390%
33	23.968	3544	3554	3561	rBV4	41288	140424	6.95%	1.176%
34	24.703	3673	3679	3686	rVB2	16587	41121	2.04%	0.344%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.850	3696	3704	3711	rBV3	25454	72614	3.59%	0.608%
36	24.926	3713	3717	3721	rVV5	11409	24465	1.21%	0.205%
37	25.008	3722	3731	3742	rVB2	178878	530926	26.28%	4.447%
38	26.066	3902	3911	3923	rVB8	11720	40549	2.01%	0.340%

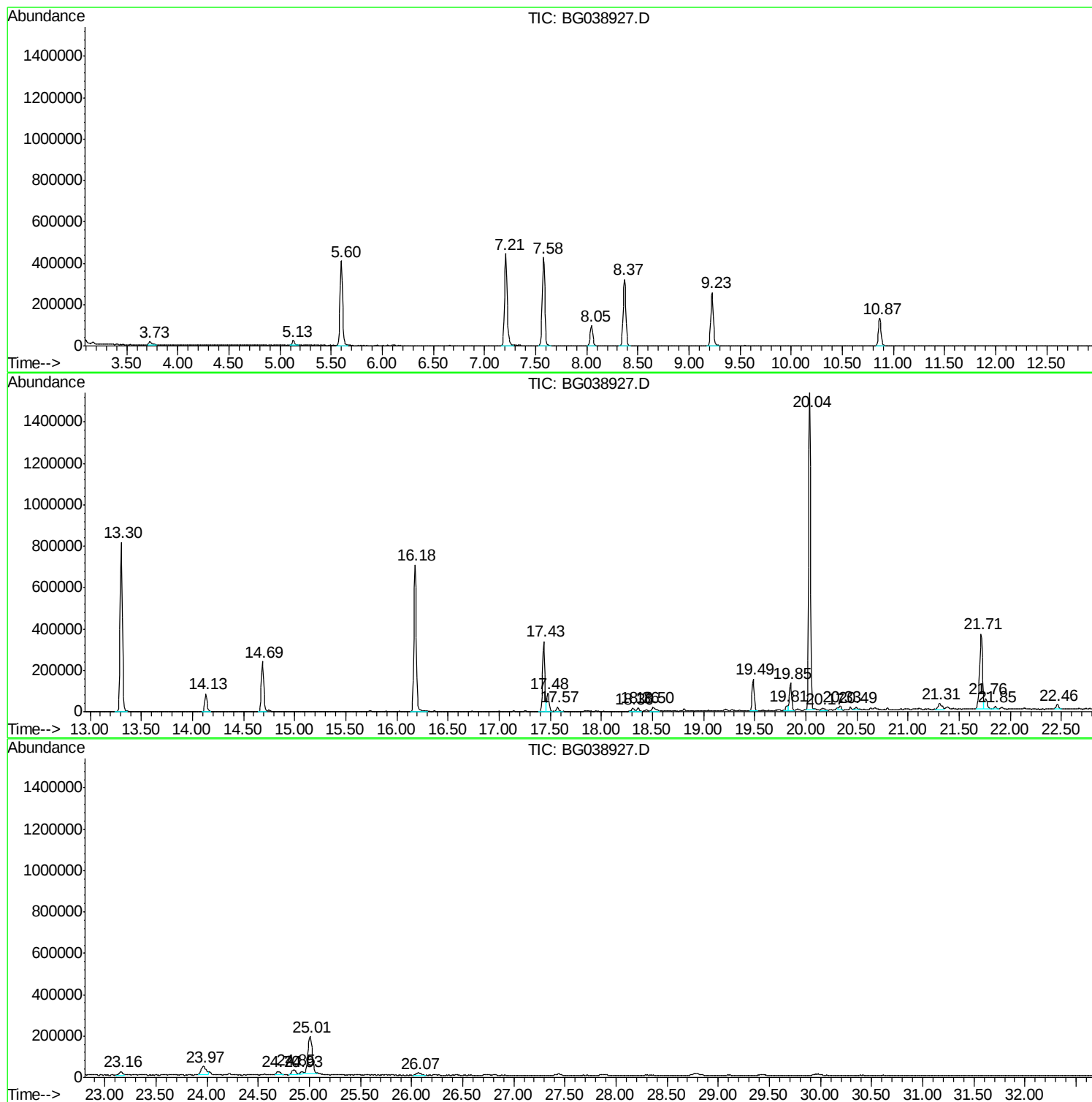
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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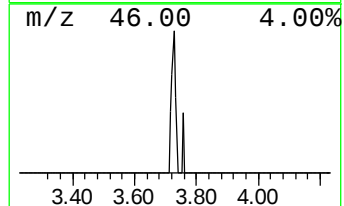
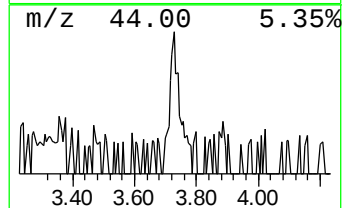
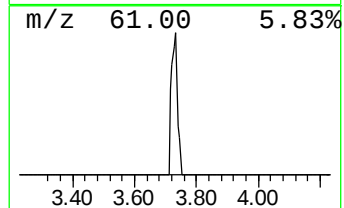
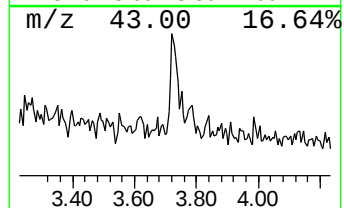
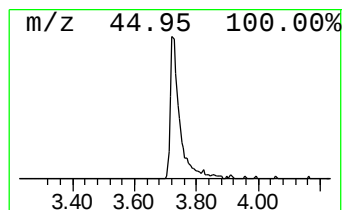
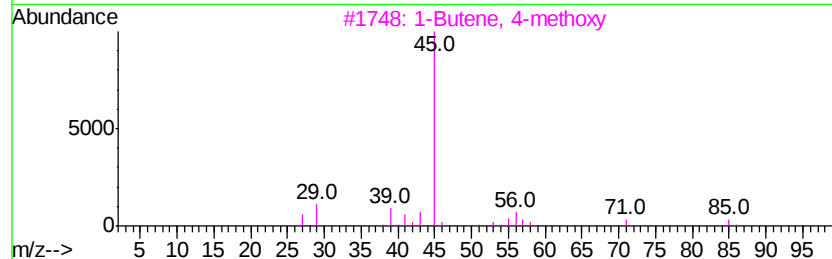
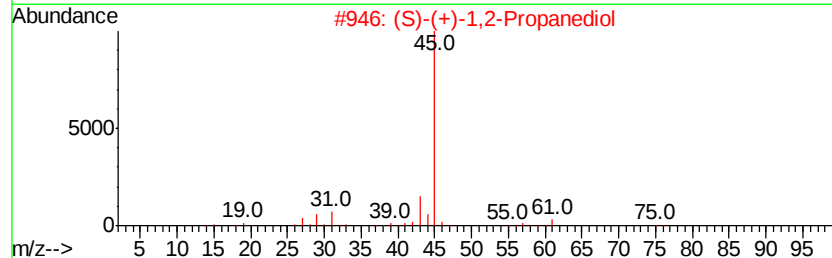
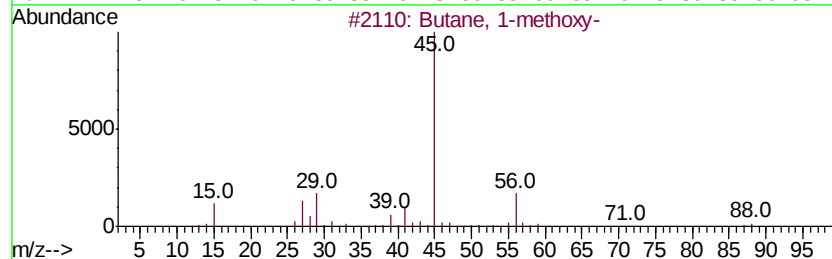
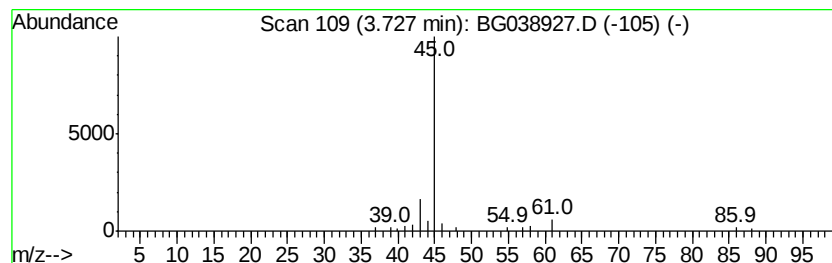
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 1-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	3.38 ng	28663	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1-methoxy-	88	C5H12O	000628-28-4	50
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
4		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9
5		2-Propanol, 1-chloro-	94	C3H7ClO	000127-00-4	9



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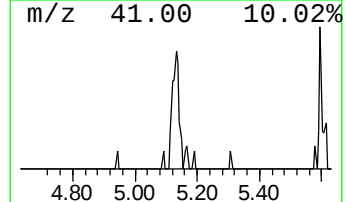
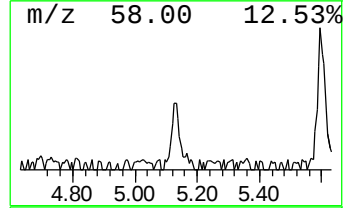
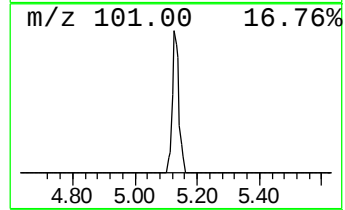
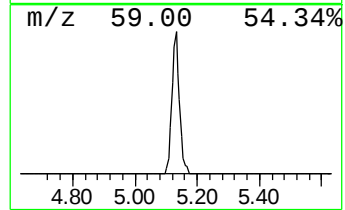
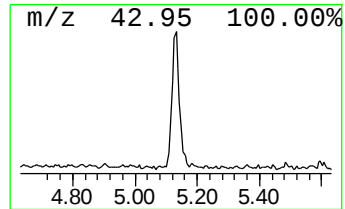
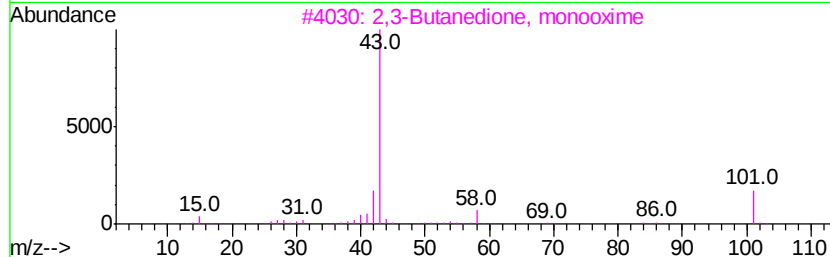
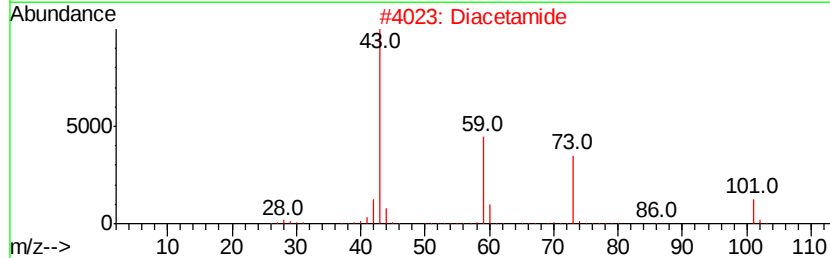
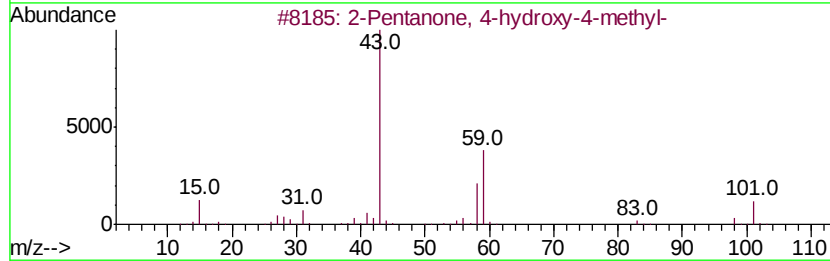
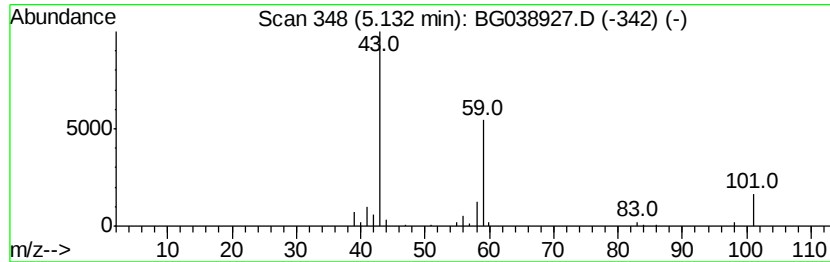
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.54 ng	38466	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Diacetamide	101	C4H7NO2	000625-77-4	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Silane, trimethyl-	74	C3H10Si	000993-07-7	9
5			3-Hexanol	102	C6H14O	000623-37-0	9



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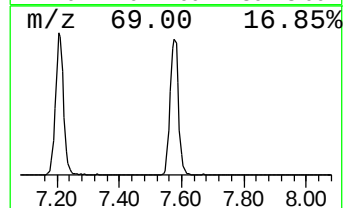
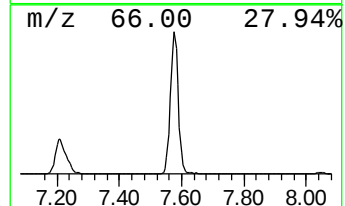
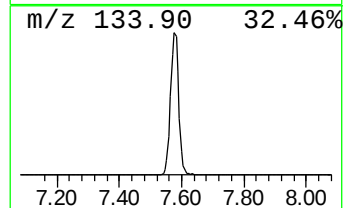
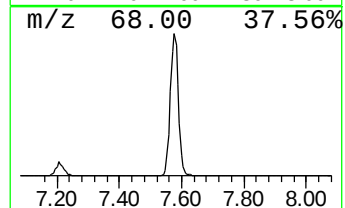
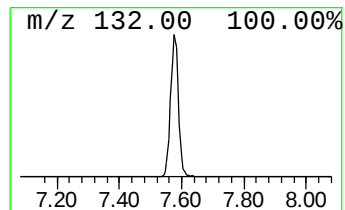
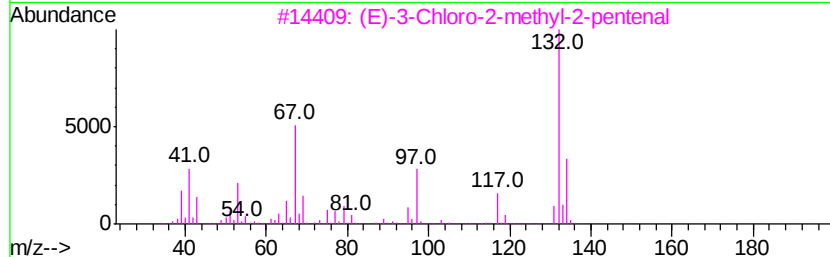
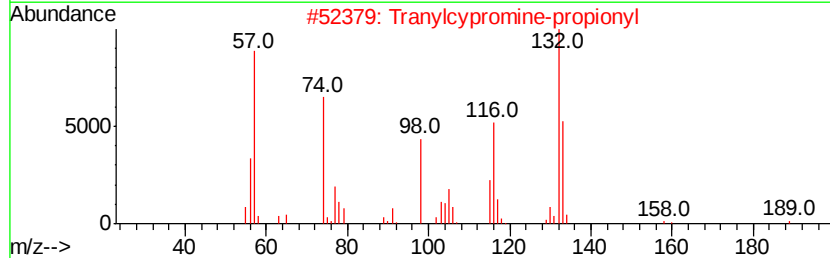
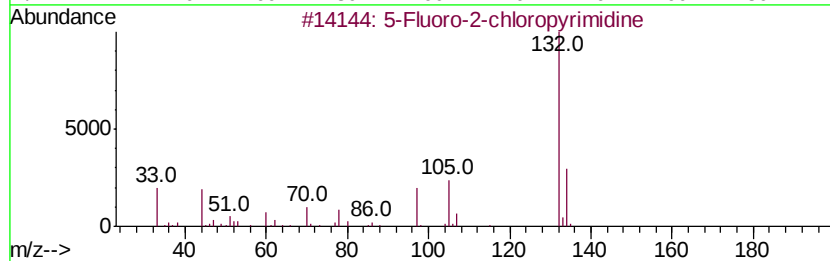
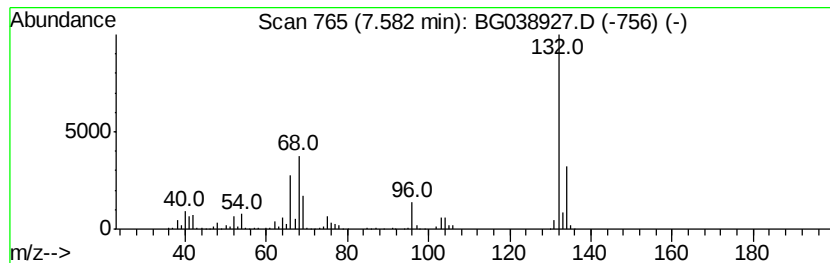
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Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	89.72 ng	760948	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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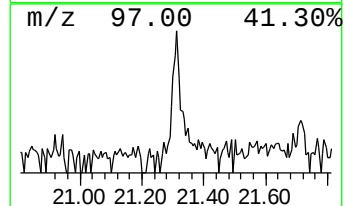
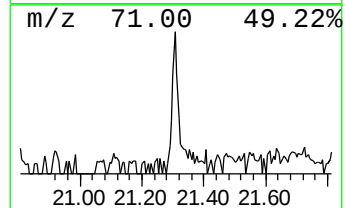
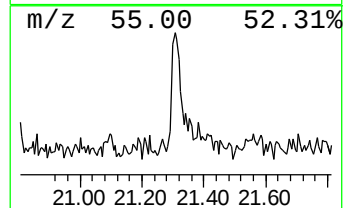
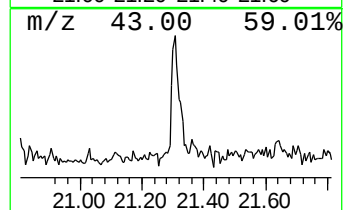
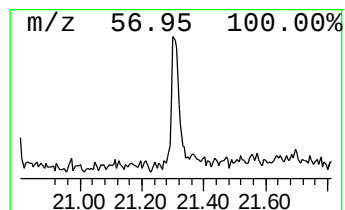
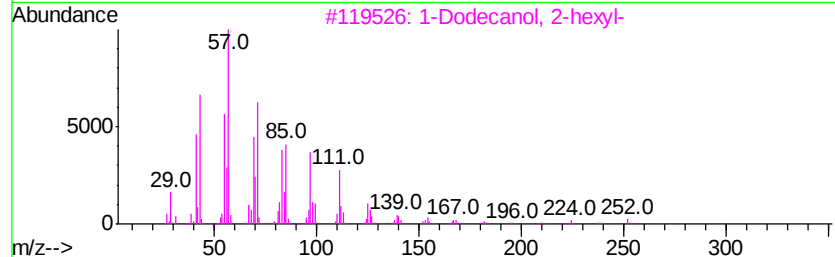
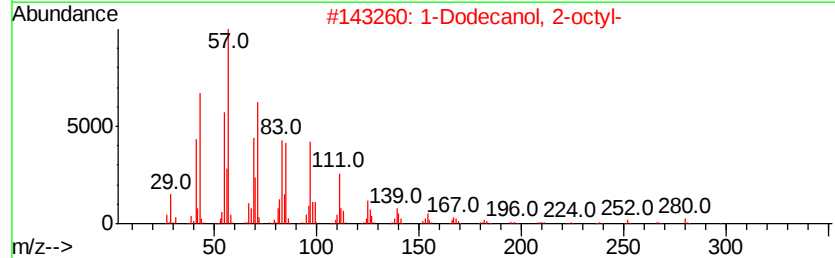
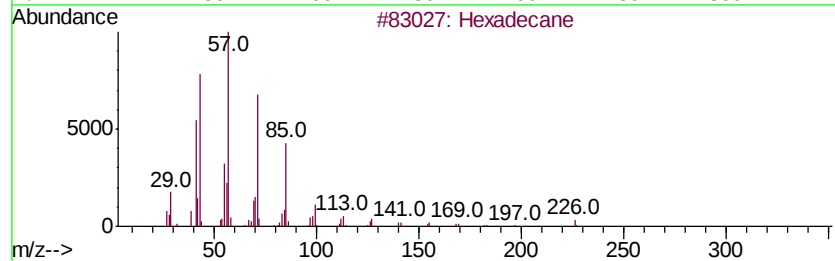
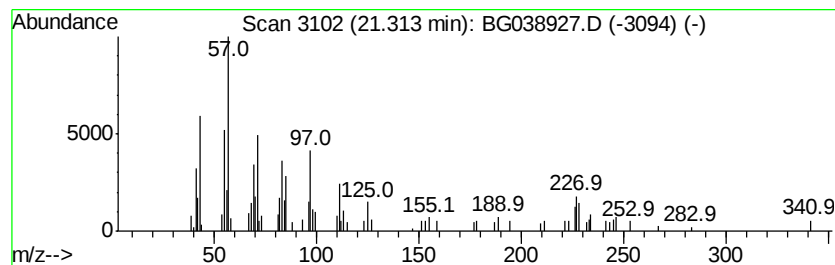
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Peak Number 5 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.08 ng	72887	Chrysene-d12	21.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	87
2	1-Dodecanol, 2-octyl-		298	C20H42O	005333-42-6	58
3	1-Dodecanol, 2-hexyl-		270	C18H38O	110225-00-8	53
4	1-Octadecanesulphonyl chloride		352	C18H37ClO2S	1000342-70-4	49
5	Triacontyl pentafluoropropionate		584	C33H61F5O2	1000351-80-0	41



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 1-methoxy-	3.73	3.4	ng	28663	1	8.05	169623	20.0
2-Pentanone, 4-hy...	5.13	4.5	ng	38466	1	8.05	169623	20.0
unknown7.58	7.58	89.7	ng	760948	1	8.05	169623	20.0
Hexadecane	21.31	2.1	ng	72887	5	21.71	701370	20.0