

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
 Data File : BG039422.D
 Acq On : 8 Feb 2019 19:15
 Operator : JU/SJ
 Sample : K1404-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A0C12-SS3-9.0-9.5

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-BG012919.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	3.226	18	23	32	rBV	87364	162009	4.23%	0.684%
2	3.296	32	35	43	rVB	57120	80710	2.11%	0.341%
3	5.252	361	368	377	rBV	89539	142367	3.71%	0.601%
4	5.711	439	446	459	rBV	1129124	1823909	47.57%	7.704%
5	7.314	710	719	733	rBV	1197149	2137645	55.76%	9.029%
6	7.702	777	785	794	rBV	1096519	1913332	49.90%	8.082%
7	8.172	858	865	878	rBV	195192	351631	9.17%	1.485%
8	8.501	912	921	930	rVB	769278	1371940	35.78%	5.795%
9	9.353	1056	1066	1075	rBV	695764	1251931	32.65%	5.288%
10	10.998	1335	1346	1354	rBV	280472	515820	13.45%	2.179%
11	13.424	1751	1759	1767	rBV	1772073	2670956	69.67%	11.282%
12	14.240	1891	1898	1904	rBV	123758	176241	4.60%	0.744%
13	14.798	1984	1993	2001	rBV2	462743	749069	19.54%	3.164%
14	16.279	2238	2245	2257	rBV	1476994	2260515	58.96%	9.548%
15	17.542	2453	2460	2473	rBV2	619100	947952	24.72%	4.004%
16	18.393	2599	2605	2615	rBV	116246	194309	5.07%	0.821%
17	19.656	2816	2820	2828	rBV2	37714	57295	1.49%	0.242%
18	20.132	2895	2901	2907	rBV	2867843	3833986	100.00%	16.194%
19	21.425	3116	3121	3132	rBV	294855	438505	11.44%	1.852%
20	21.830	3183	3190	3199	rVB	689959	1129455	29.46%	4.771%
21	22.623	3320	3325	3329	rBV3	23396	41839	1.09%	0.177%
22	23.351	3443	3449	3459	rVB3	29132	59744	1.56%	0.252%
23	24.191	3587	3592	3601	rVB4	30961	64102	1.67%	0.271%
24	25.214	3754	3766	3782	rBV	386982	1156632	30.17%	4.885%
25	26.400	3961	3968	3978	rVB3	21784	58671	1.53%	0.248%
26	26.541	3984	3992	4002	rBV7	24168	84505	2.20%	0.357%

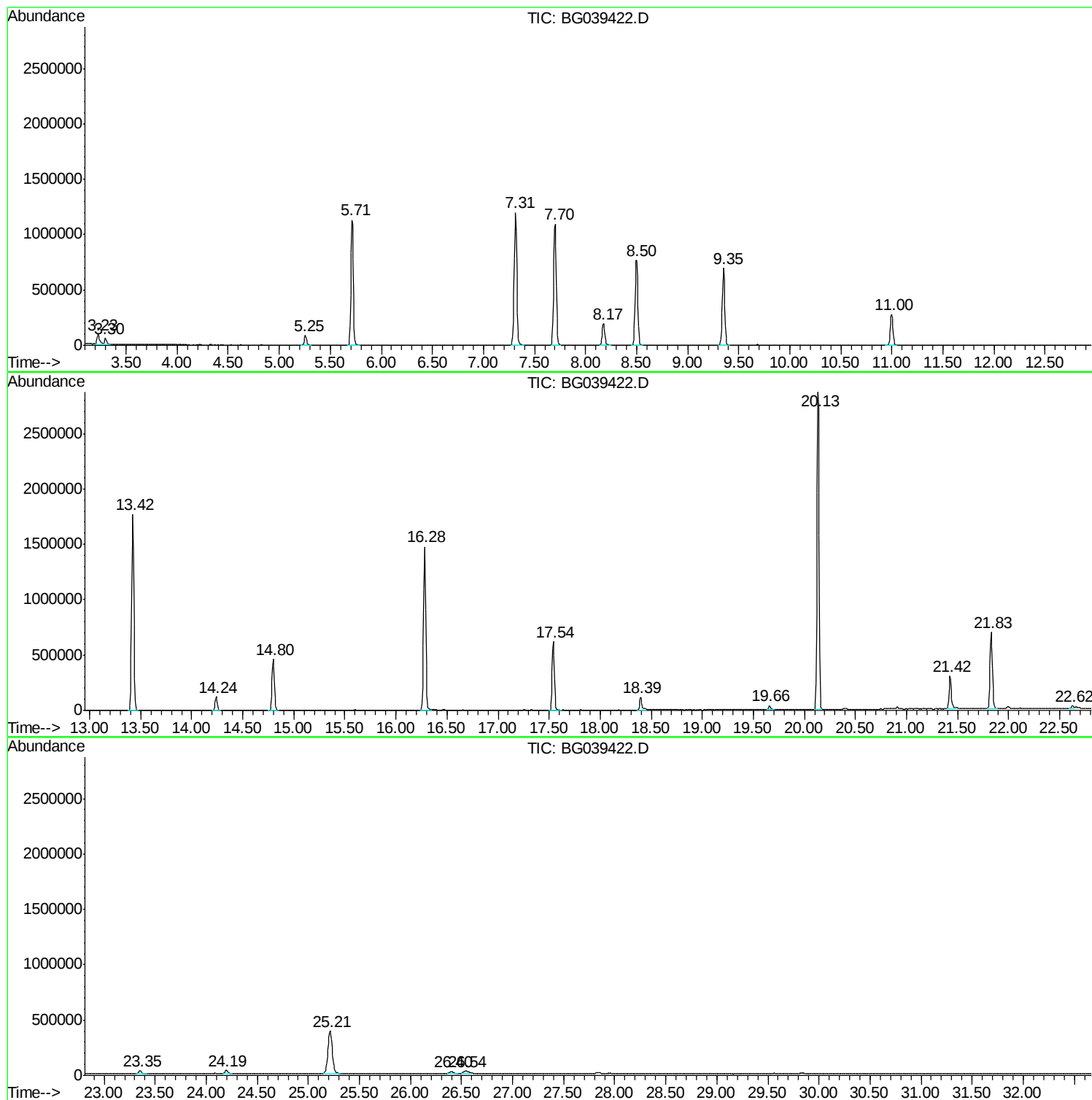
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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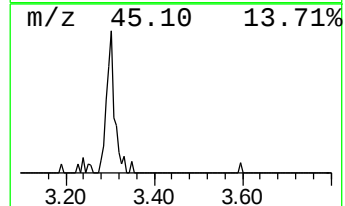
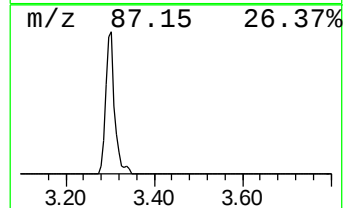
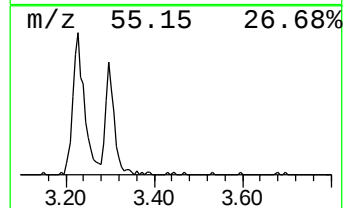
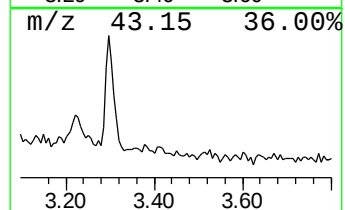
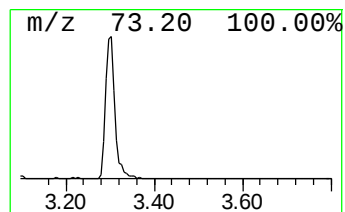
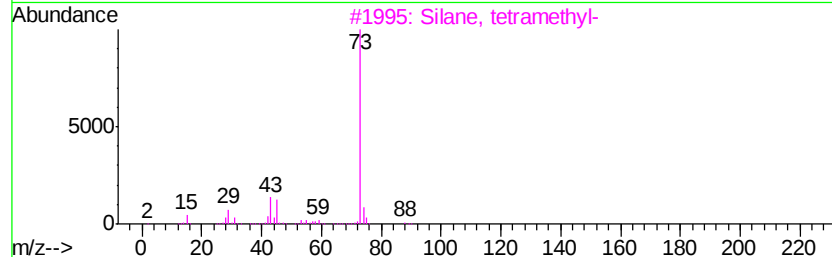
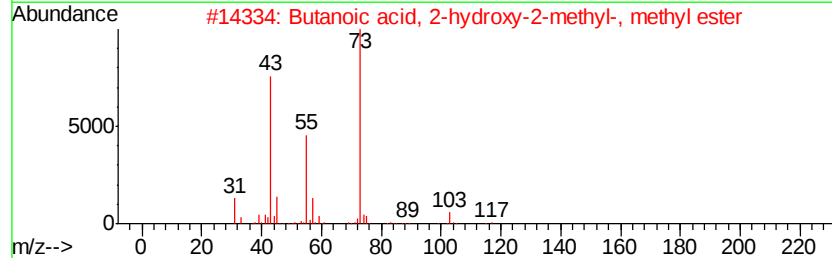
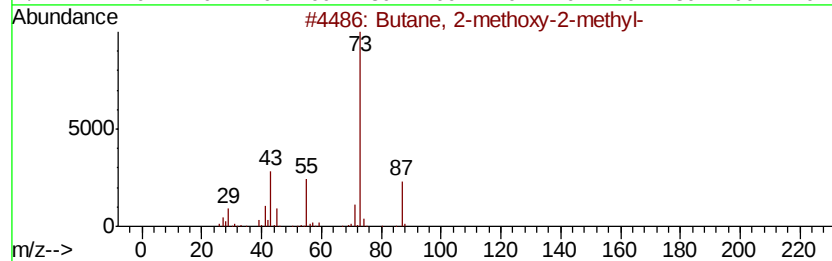
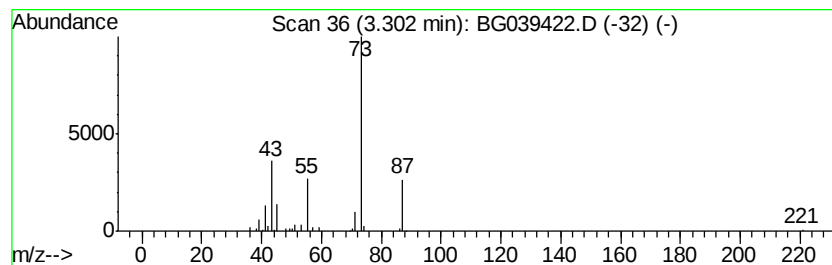
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	4.59 ng	80710	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	17
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	10



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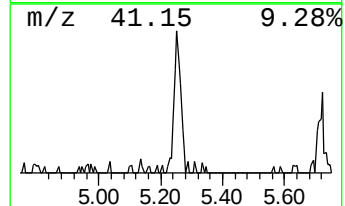
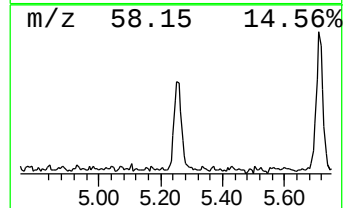
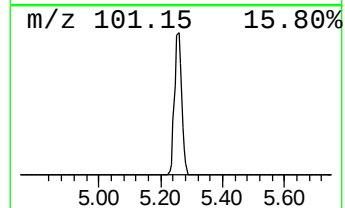
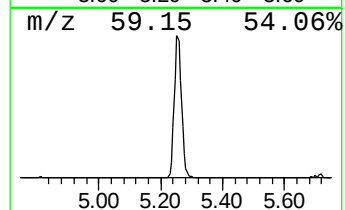
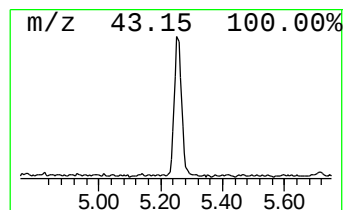
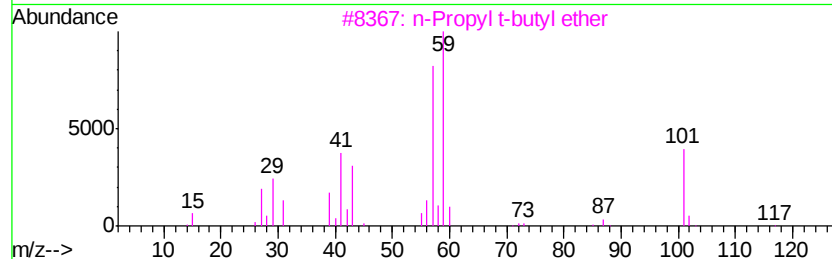
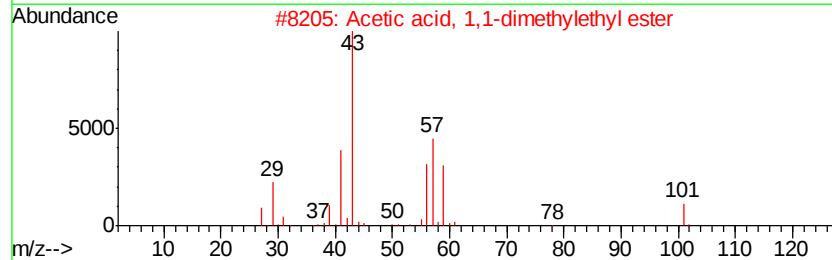
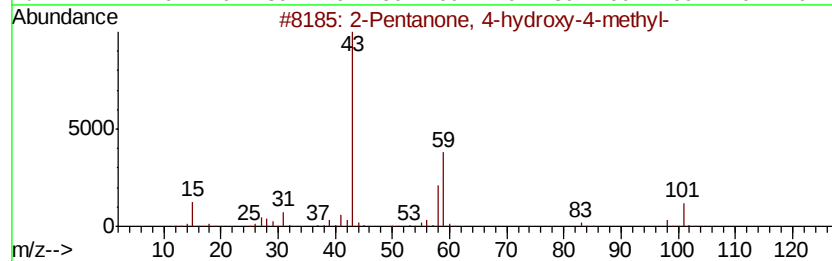
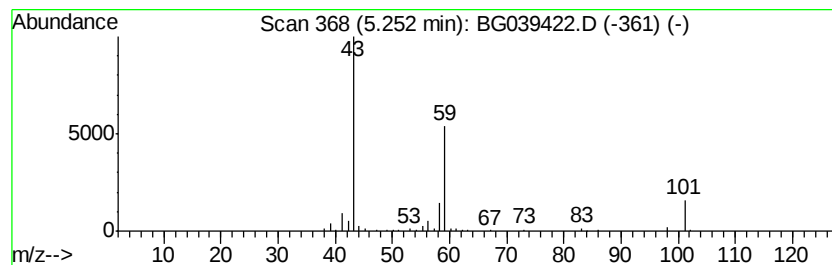
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	8.10 ng	142367	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	37
3			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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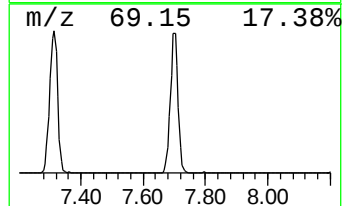
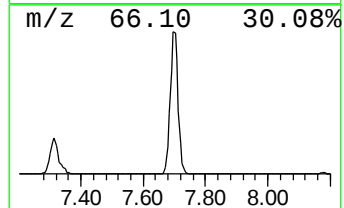
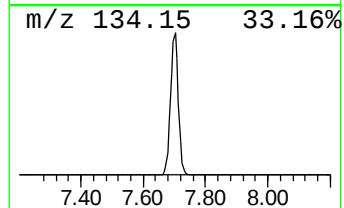
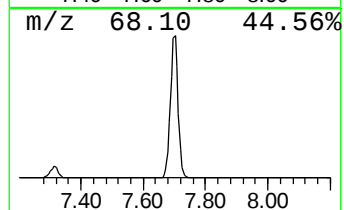
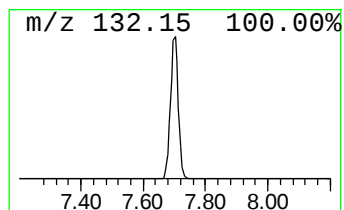
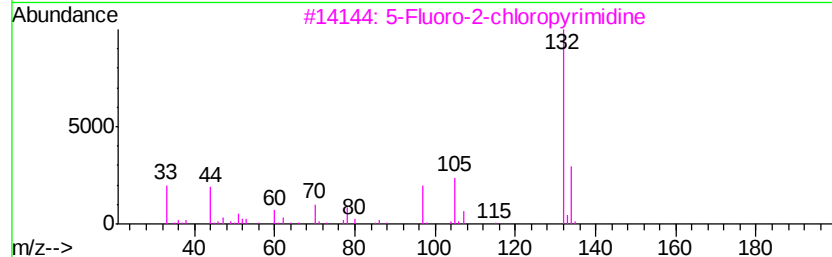
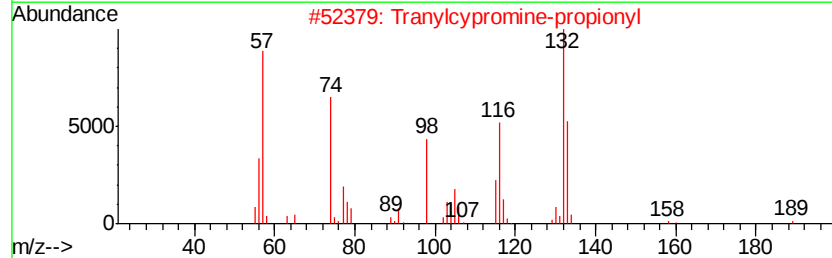
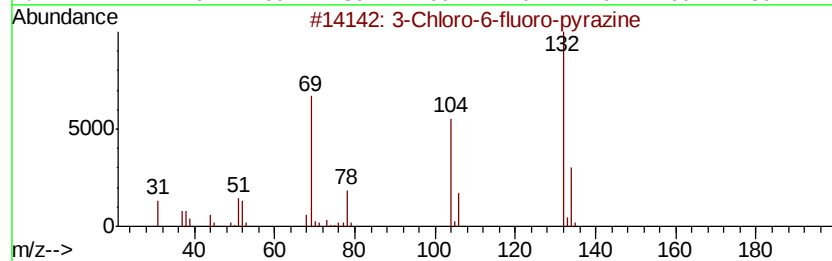
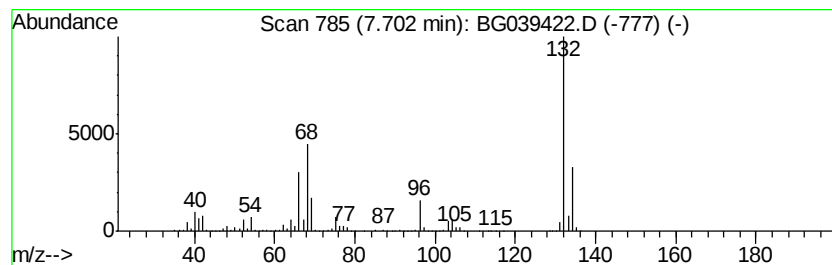
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Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	108.83 ng	1913330	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Xenon	132	Xe	007440-63-3	9



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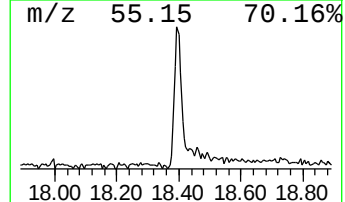
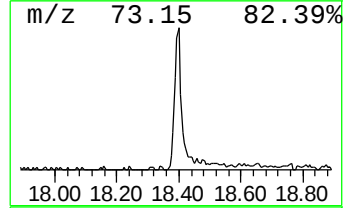
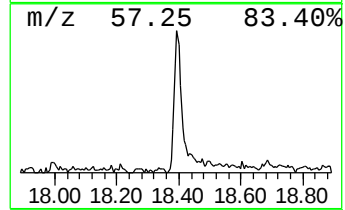
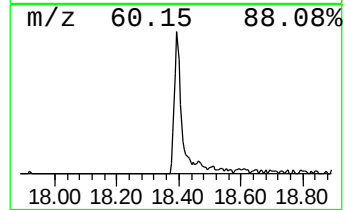
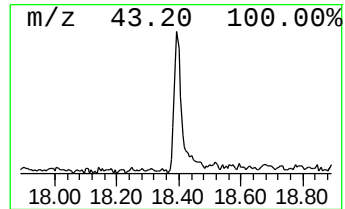
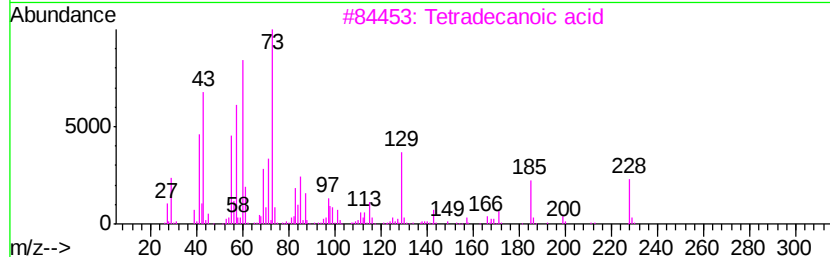
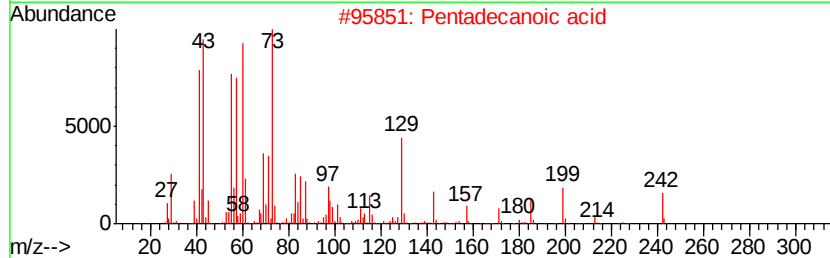
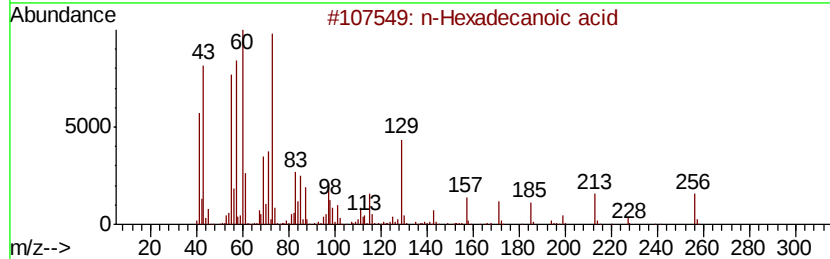
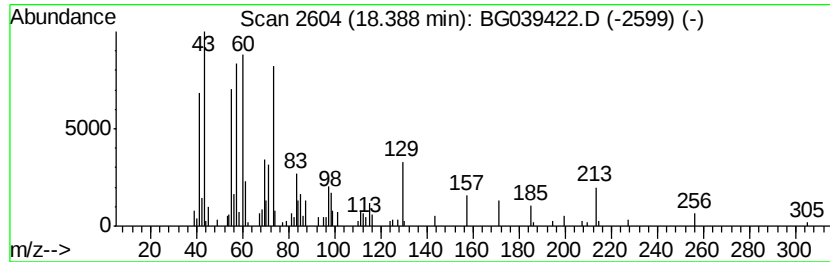
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	4.10 ng	194309	Phenanthrene-d10	17.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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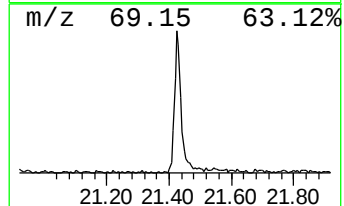
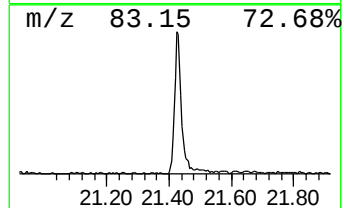
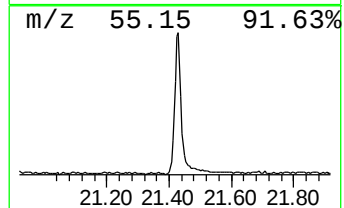
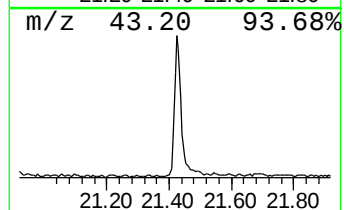
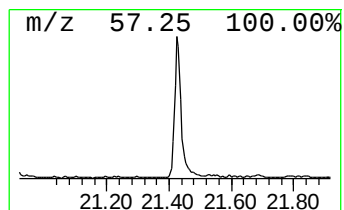
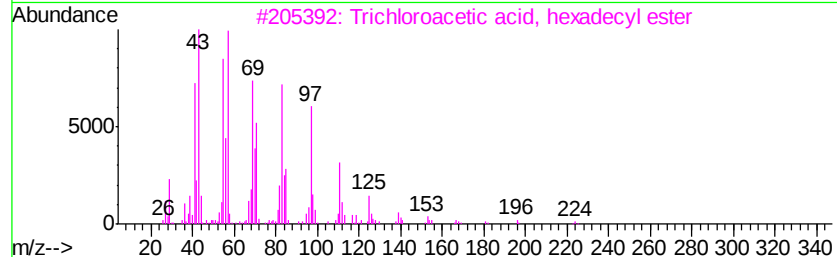
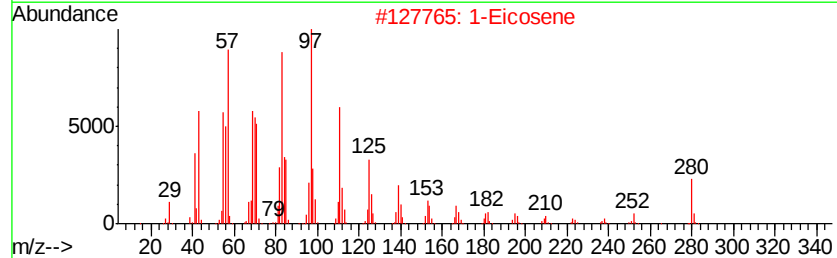
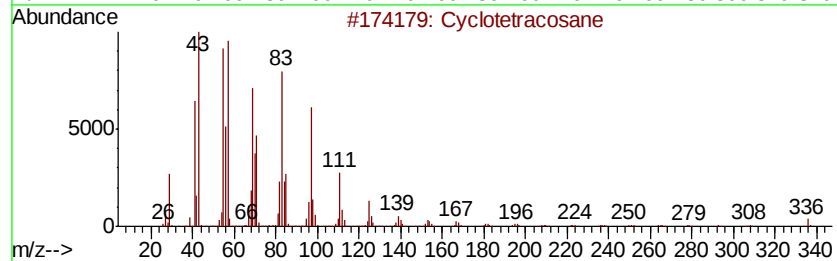
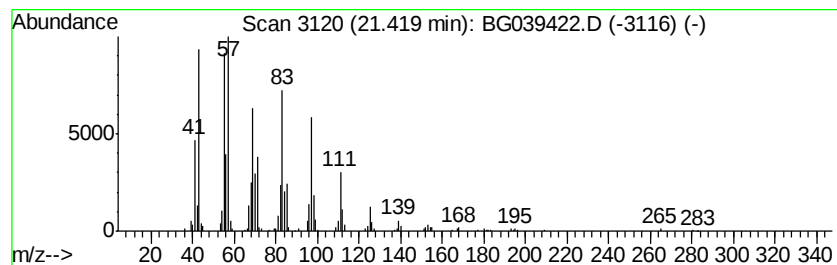
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Peak Number 7 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	7.76 ng	438505	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetracosane	336	C24H48	000297-03-0	95
2		1-Eicosene	280	C20H40	003452-07-1	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.30	4.6	ng	80710	1	8.17	351631	20.0
2-Pentanone, 4-hy...	5.25	8.1	ng	142367	1	8.17	351631	20.0
unknown7.70	7.70	108.8	ng	1913330	1	8.17	351631	20.0
n-Hexadecanoic acid	18.39	4.1	ng	194309	4	17.54	947952	20.0
Cyclotetracosane	21.42	7.8	ng	438505	5	21.83	1129460	20.0