

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
 Data File : BG039418.D
 Acq On : 8 Feb 2019 16:39
 Operator : JU/SJ
 Sample : K1404-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A0C12-SS1-7.5-8.0

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	3.225	18	23	32	rBV2	79687	150075	3.35%	0.574%
2	3.295	32	35	46	rVB	59167	85235	1.91%	0.326%
3	5.257	363	369	376	rBV	75200	120007	2.68%	0.459%
4	5.716	439	447	459	rBV	1263623	2032671	45.44%	7.772%
5	7.314	710	719	731	rBV	1324179	2468517	55.18%	9.438%
6	7.701	777	785	793	rBV	1252097	2139750	47.83%	8.181%
7	8.177	858	866	877	rBV	211595	375177	8.39%	1.434%
8	8.500	913	921	929	rBV	807123	1433713	32.05%	5.482%
9	9.352	1058	1066	1076	rBV	757807	1375028	30.74%	5.257%
10	10.997	1339	1346	1354	rBV	300150	538827	12.04%	2.060%
11	13.423	1750	1759	1772	rBV	1859716	2868262	64.11%	10.967%
12	14.239	1892	1898	1905	rBV	166275	242945	5.43%	0.929%
13	14.798	1986	1993	2002	rVB2	511896	803653	17.96%	3.073%
14	16.284	2239	2246	2263	rBV	1611210	2574055	57.54%	9.842%
15	17.541	2454	2460	2466	rBV2	668570	1022918	22.86%	3.911%
16	18.399	2601	2606	2619	rBV2	62318	122488	2.74%	0.468%
17	20.137	2895	2902	2908	rBV	3338281	4473787	100.00%	17.105%
18	20.907	3029	3033	3038	rVB2	36691	46002	1.03%	0.176%
19	21.430	3116	3122	3134	rBV	163491	271686	6.07%	1.039%
20	21.829	3183	3190	3199	rBV	744687	1225058	27.38%	4.684%
21	21.994	3211	3218	3224	rBV	53922	80512	1.80%	0.308%
22	22.628	3320	3326	3337	rBV	52266	98488	2.20%	0.377%
23	23.351	3443	3449	3458	rBV3	54849	106030	2.37%	0.405%
24	24.202	3586	3594	3604	rVB	56265	121932	2.73%	0.466%
25	25.213	3755	3766	3786	rBV3	408321	1284648	28.72%	4.912%
26	26.405	3959	3969	3978	rVB4	32303	93036	2.08%	0.356%

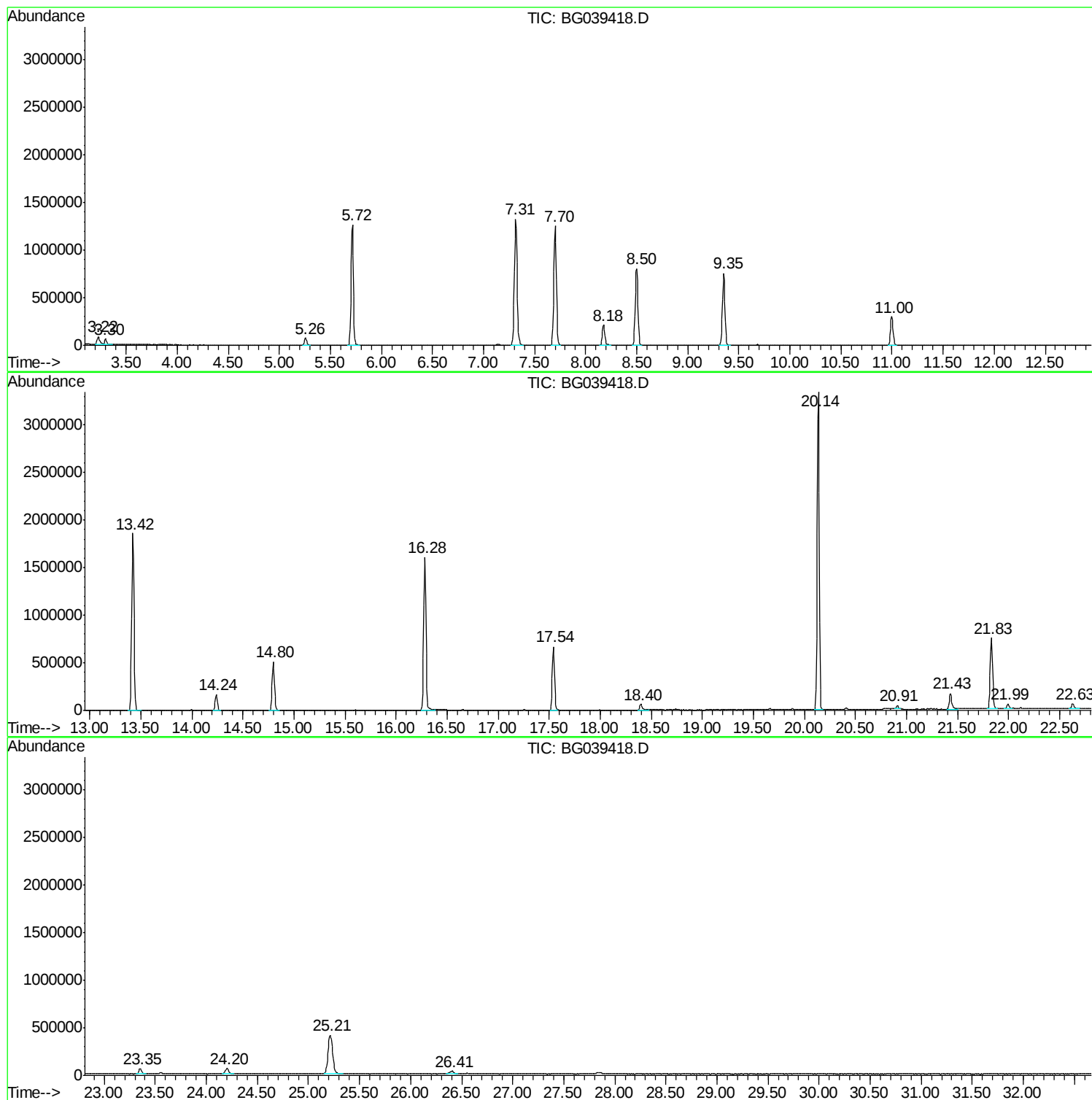
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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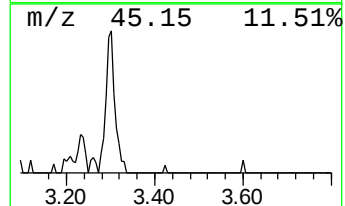
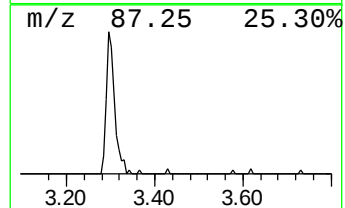
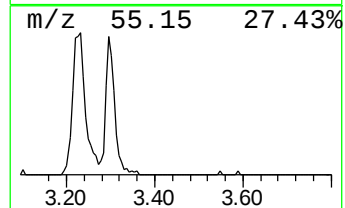
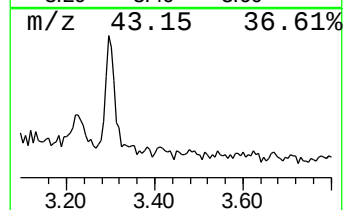
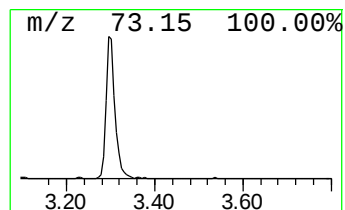
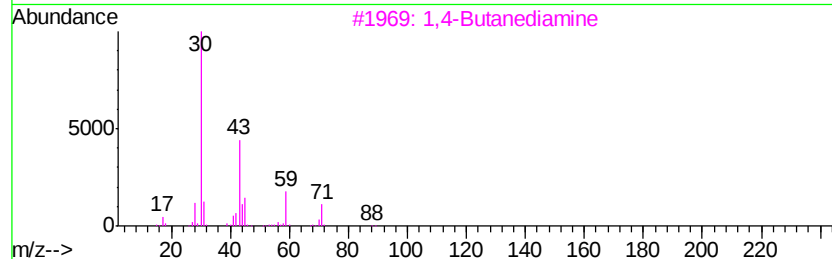
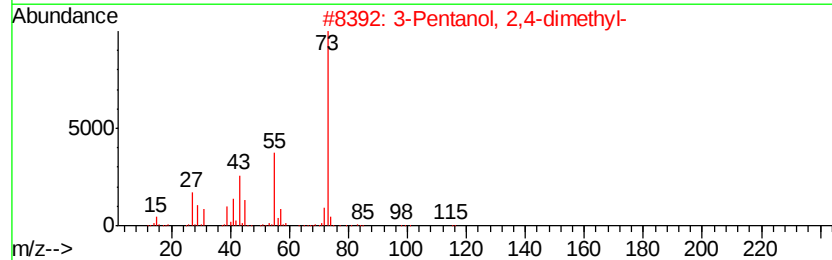
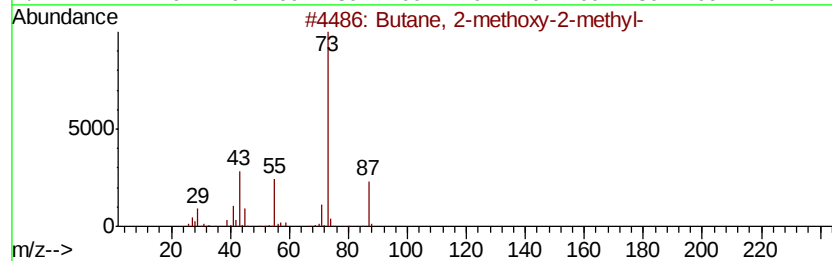
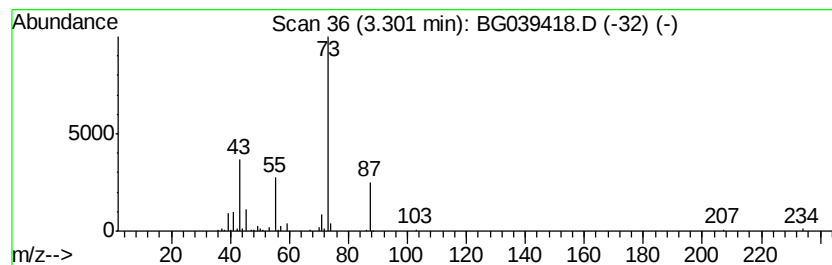
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	4.54 ng	85235	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
3		1,4-Butanediamine	88	C4H12N2	000110-60-1	12
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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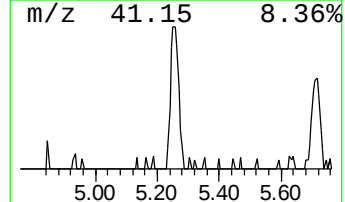
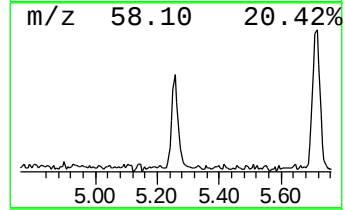
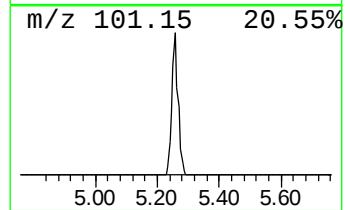
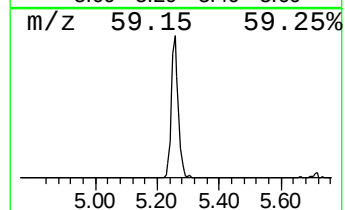
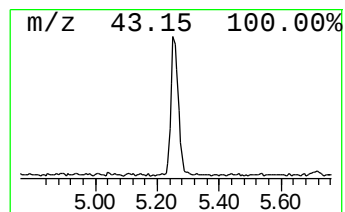
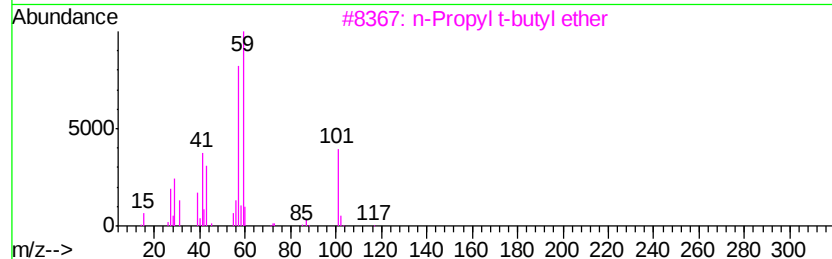
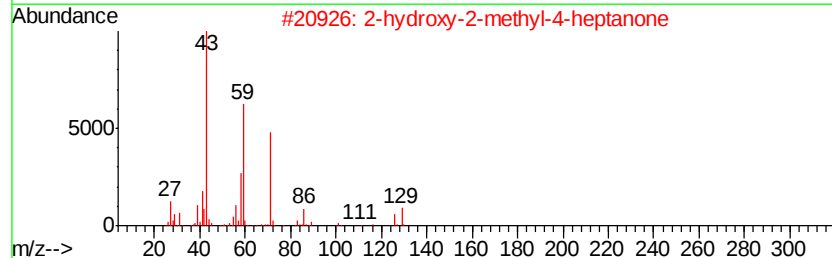
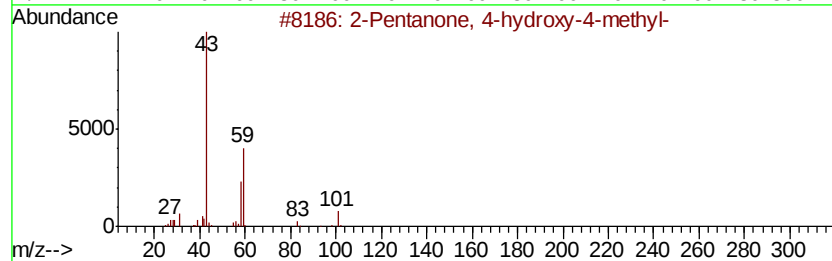
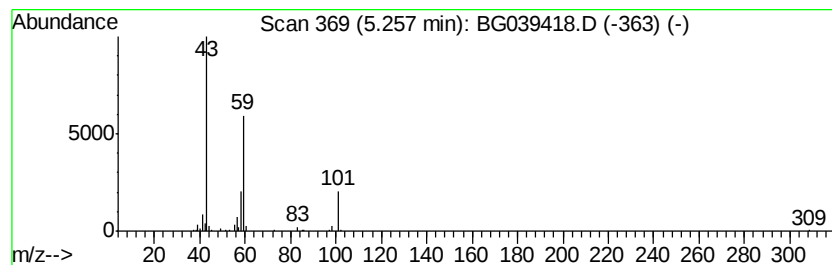
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.26	6.40 ng	120007	1,4-Dichlorobenzene-d4	8.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	45
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12



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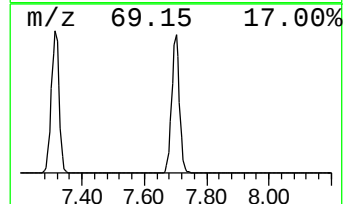
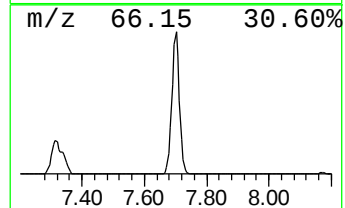
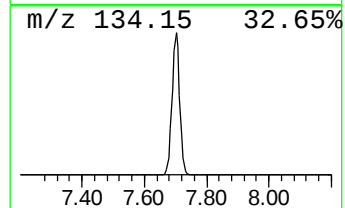
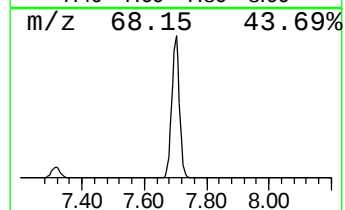
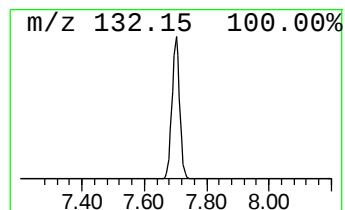
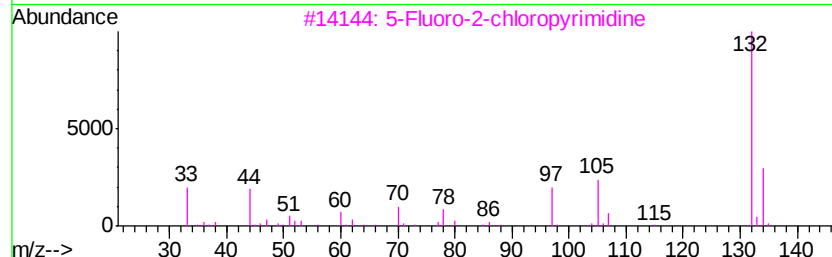
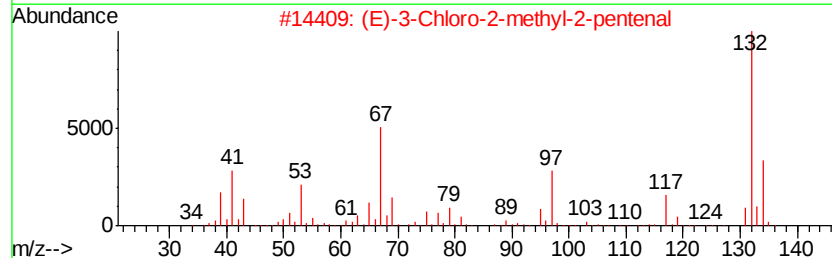
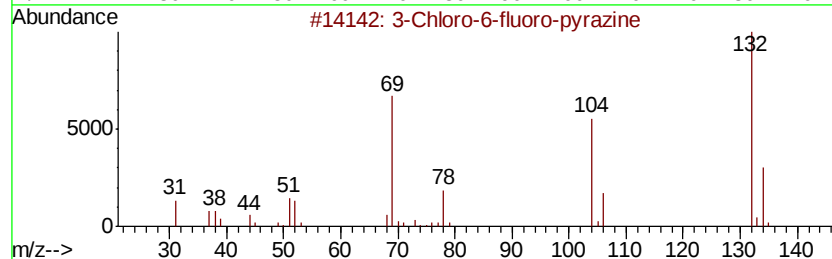
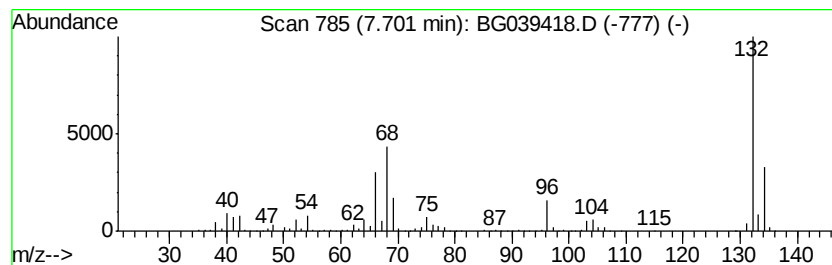
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Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	114.07 ng	2139750	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9



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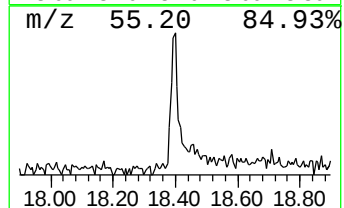
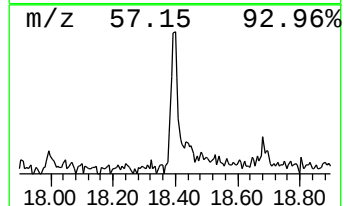
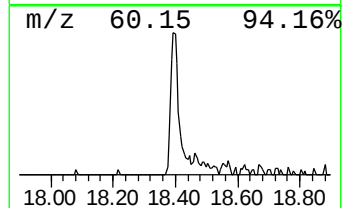
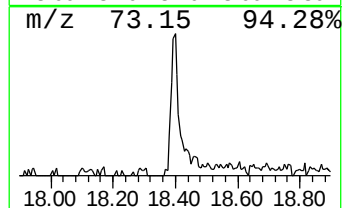
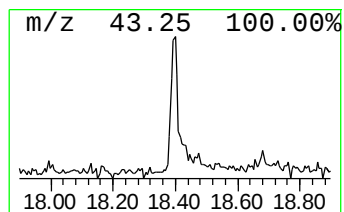
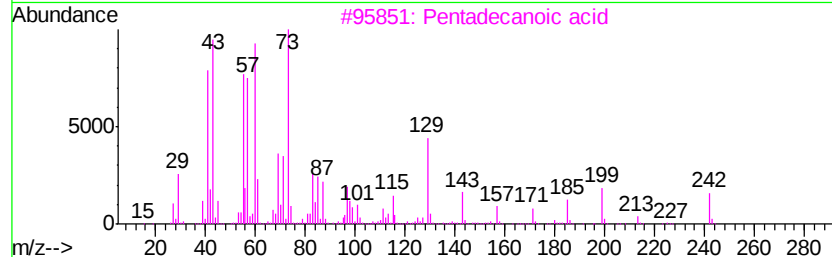
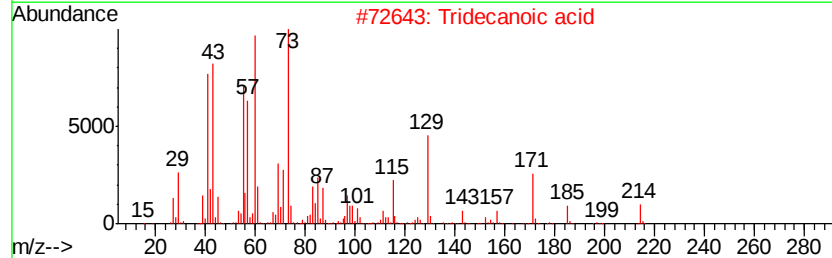
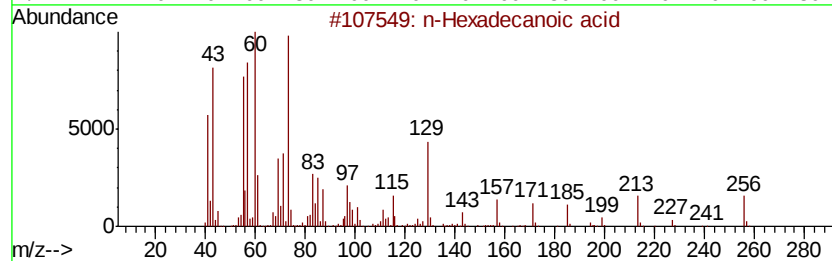
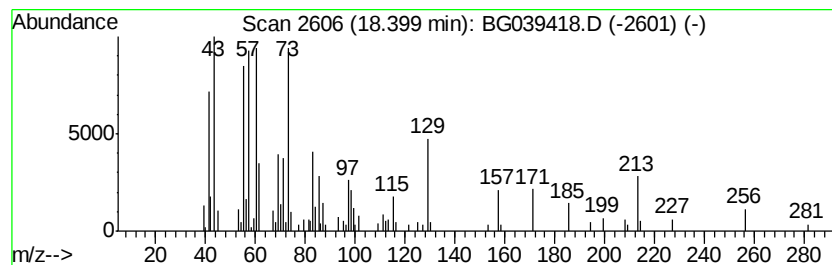
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.40	2.39 ng	122488	Phenanthrene-d10		17.54
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38



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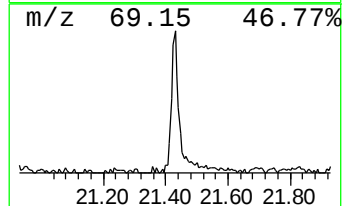
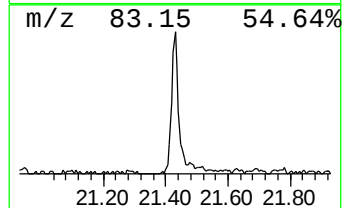
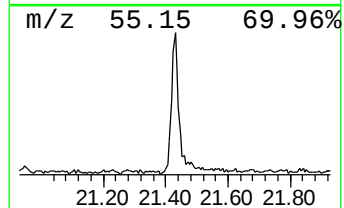
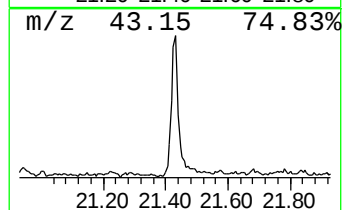
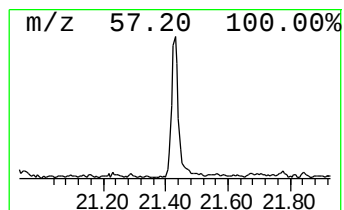
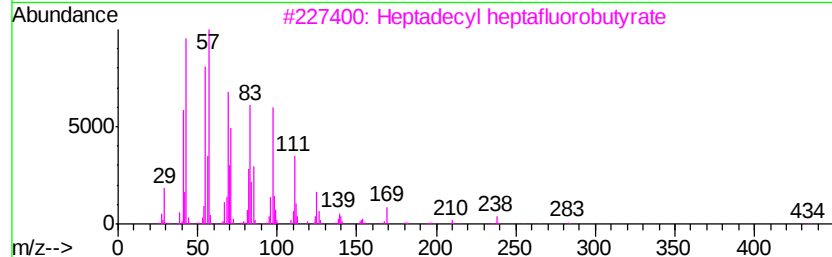
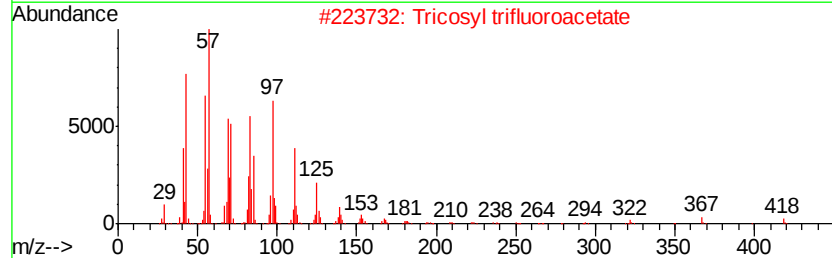
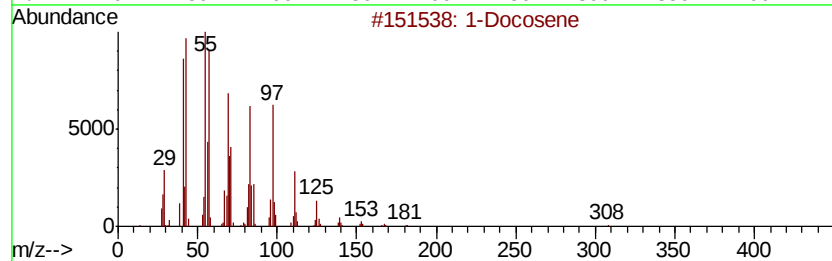
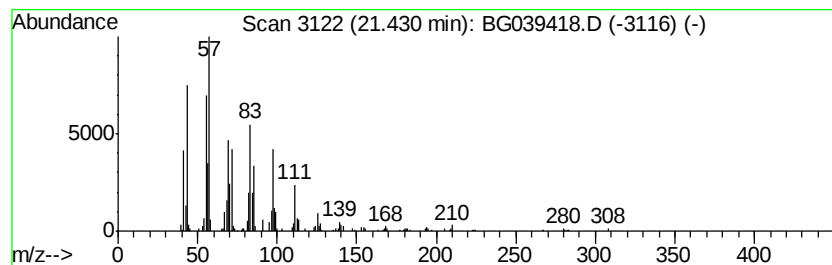
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Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	4.44 ng	271686	Chrysene-d12	21.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	99
2	Tricosyl trifluoroacetate	436 C25H47F3O2	1000351-75-1	91
3	Heptadecyl heptafluorobutyrat	452 C21H35F7O2	959085-66-6	91
4	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	91
5	3-Eicosene, (E)-	280 C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.30	4.5	ng	85235	1	8.18	375177	20.0
2-Pentanone, 4-hy...	5.26	6.4	ng	120007	1	8.18	375177	20.0
unknown7.70	7.70	114.1	ng	2139750	1	8.18	375177	20.0
n-Hexadecanoic acid	18.40	2.4	ng	122488	4	17.54	1022920	20.0
1-Docosene	21.43	4.4	ng	271686	5	21.83	1225060	20.0