

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
 Data File : BG042971.D
 Acq On : 1 Oct 2019 17:43
 Operator : JU
 Sample : K4946-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GP-4 (1-3)

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-BG092519.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	3.184	9	16	24	rBV3	90266	225373	6.05%	1.018%
2	3.260	25	29	42	rVB2	64716	120510	3.23%	0.544%
3	5.651	429	436	446	rBV	837045	1407971	37.77%	6.358%
4	7.238	698	706	724	rBV	928655	1700142	45.61%	7.677%
5	7.608	761	769	779	rBV	907296	1559424	41.83%	7.042%
6	8.072	841	848	857	rBV	243818	438978	11.78%	1.982%
7	8.395	892	903	913	rBV	641766	1146056	30.74%	5.175%
8	9.230	1036	1045	1055	rBV	525186	994955	26.69%	4.493%
9	10.875	1313	1325	1334	rBV	321725	597996	16.04%	2.700%
10	13.313	1732	1740	1754	rBV	1380398	2174214	58.33%	9.818%
11	14.136	1874	1880	1887	rBV	218599	312567	8.39%	1.411%
12	14.688	1966	1974	1984	rBV	558408	879908	23.61%	3.973%
13	16.174	2219	2227	2242	rBV	1410584	2138739	57.38%	9.658%
14	17.432	2434	2441	2452	rBV	734794	1142116	30.64%	5.157%
15	18.319	2587	2592	2601	rBV	106214	150038	4.03%	0.678%
16	20.040	2878	2885	2892	rBV	2652109	3727623	100.00%	16.832%
17	21.345	3103	3107	3122	rBV2	122858	360089	9.66%	1.626%
18	21.697	3161	3167	3175	rBV2	825877	1411412	37.86%	6.373%
19	23.401	3453	3457	3463	rVB3	46853	92188	2.47%	0.416%
20	24.923	3707	3716	3732	rVB2	495433	1519211	40.76%	6.860%
21	26.098	3910	3916	3917	rBV5	30834	46192	1.24%	0.209%

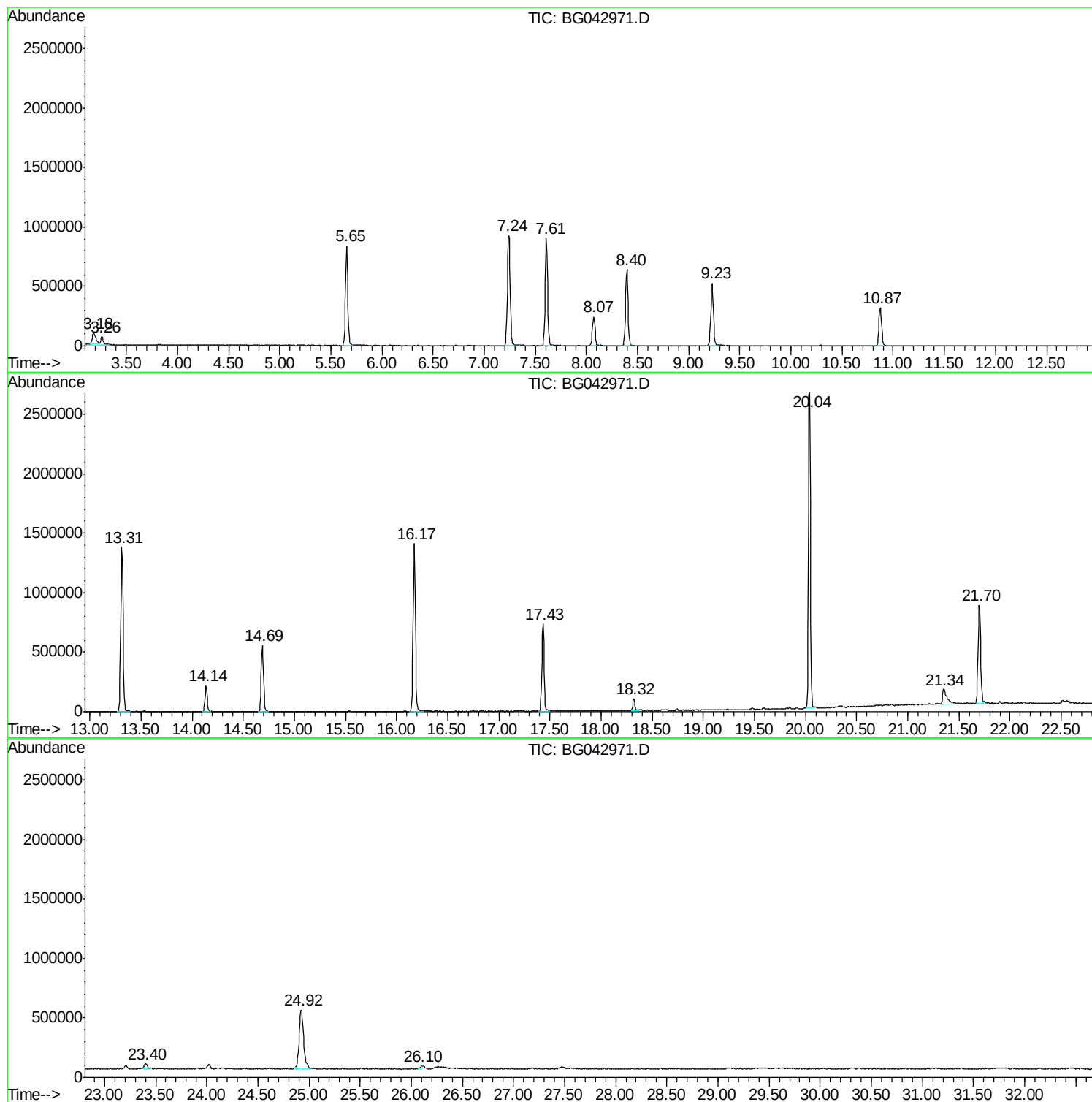
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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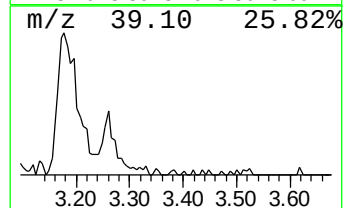
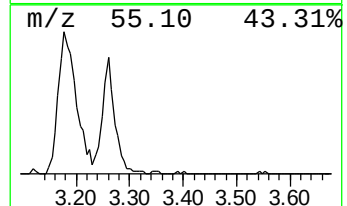
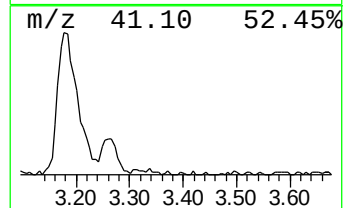
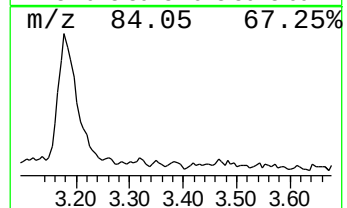
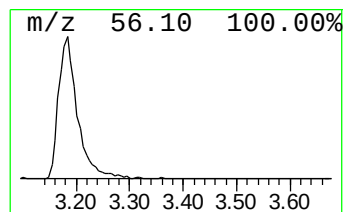
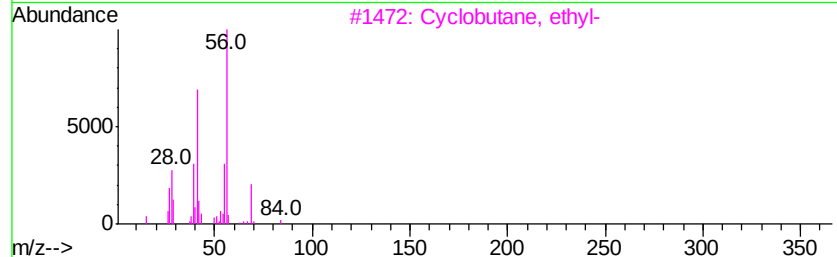
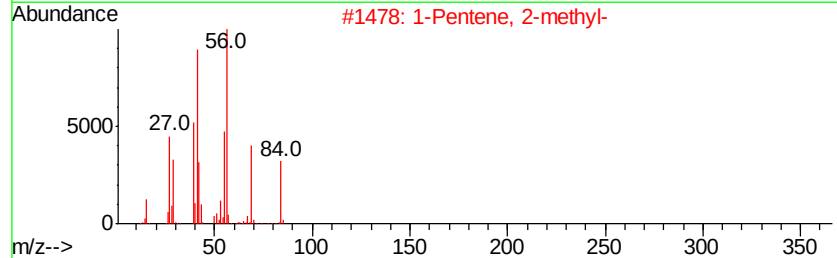
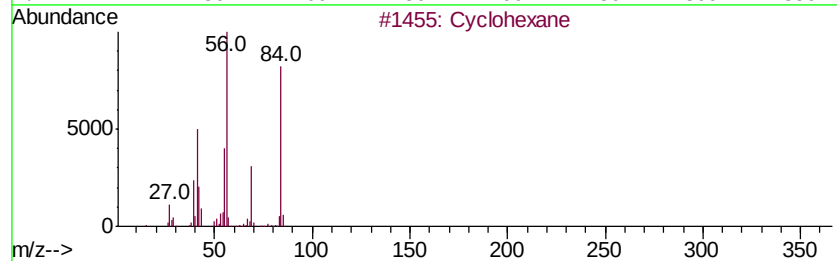
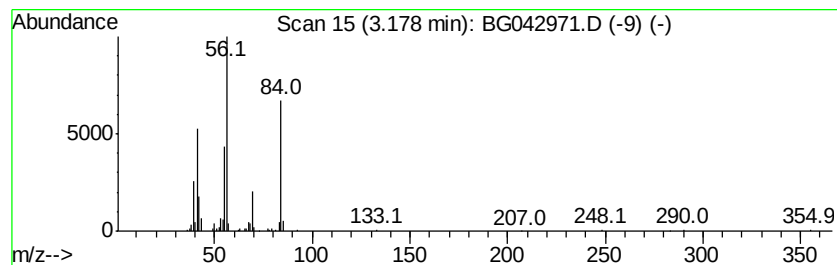
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092519.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	10.27 ng	225373	1,4-Dichlorobenzene-d4	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane	84	C6H12	000110-82-7	91
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
4		Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	43
5		Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	42



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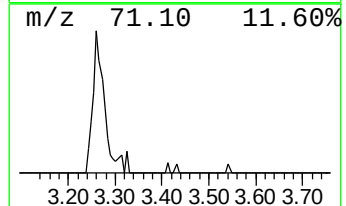
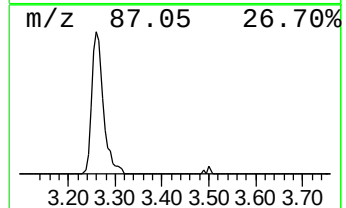
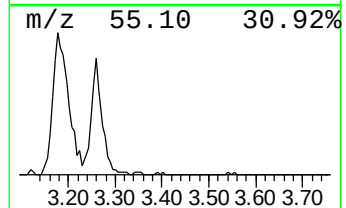
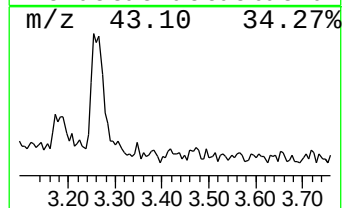
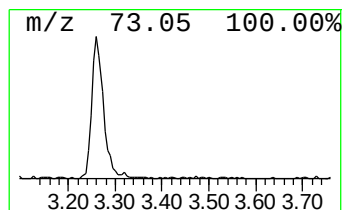
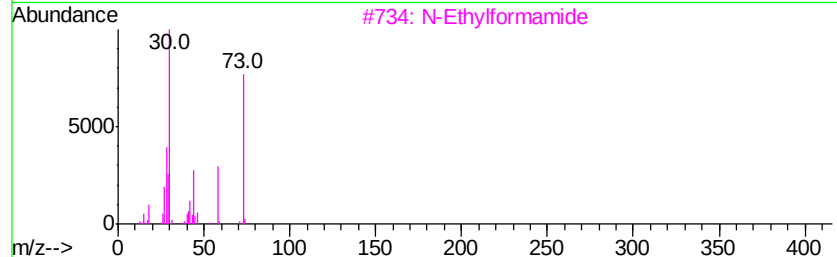
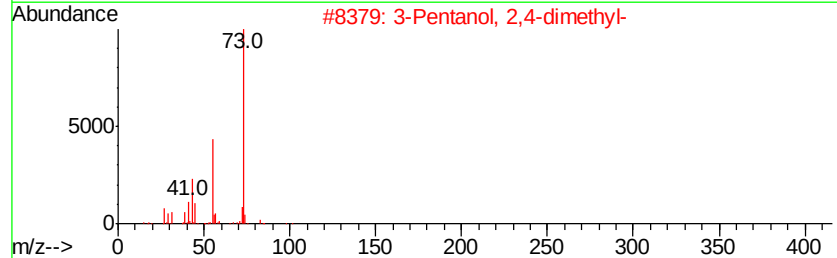
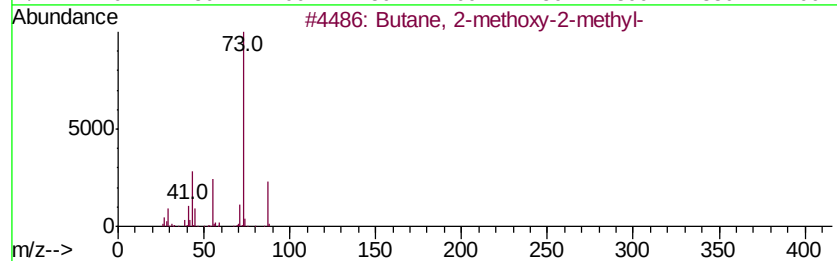
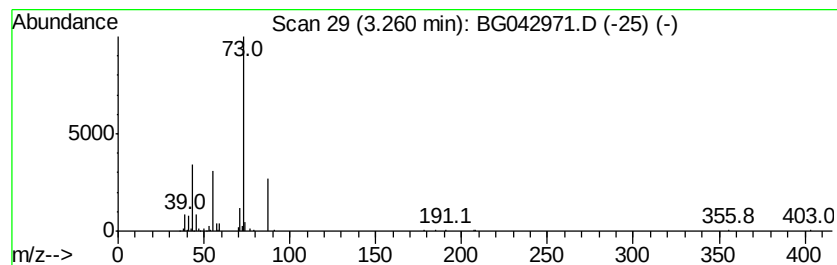
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	5.49 ng	120510	1,4-Dichlorobenzene-d4	8.07

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	10
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	9



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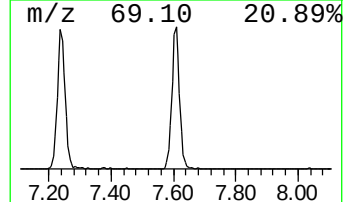
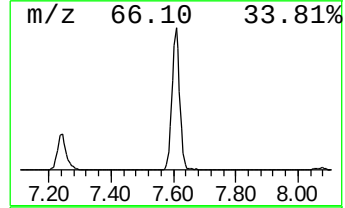
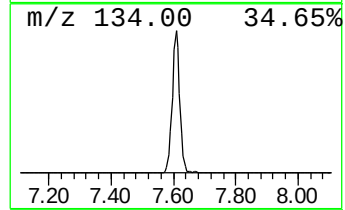
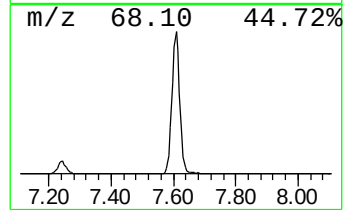
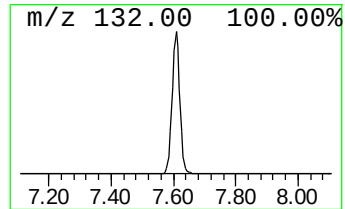
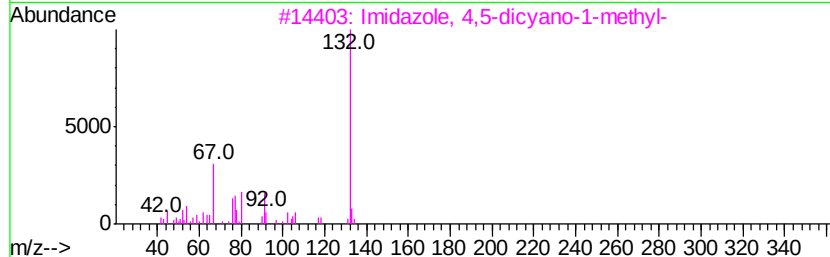
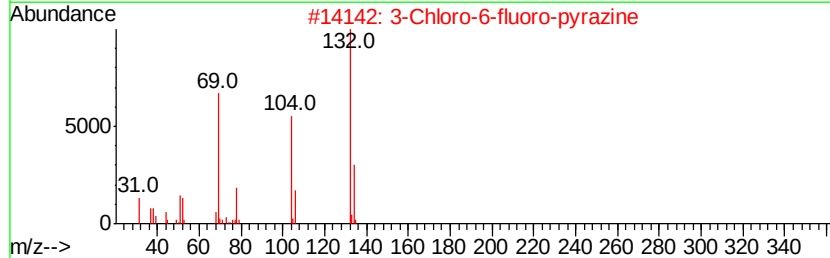
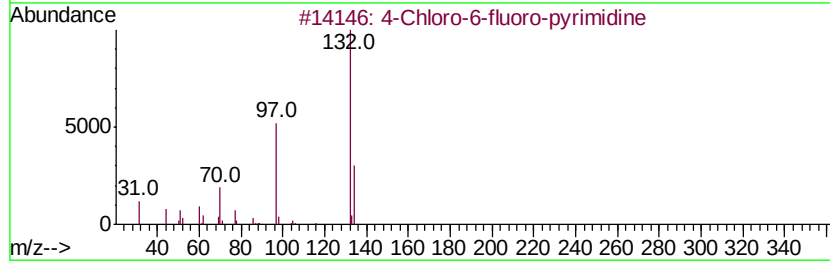
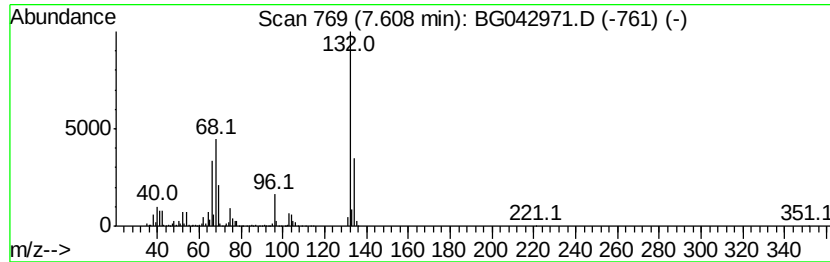
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Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	71.05 ng	1559420	1,4-Dichlorobenzene-d4	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22



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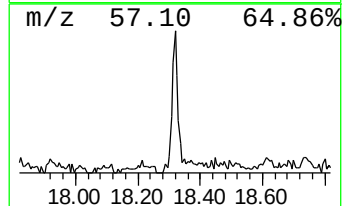
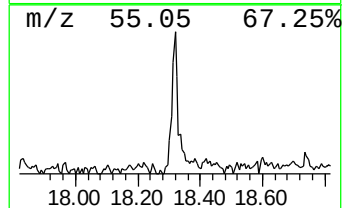
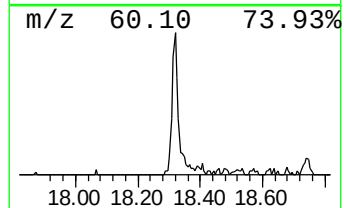
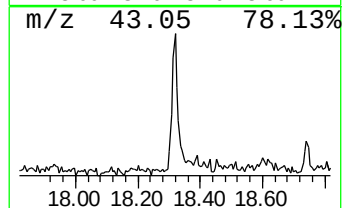
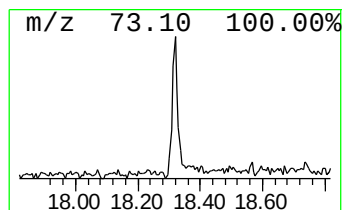
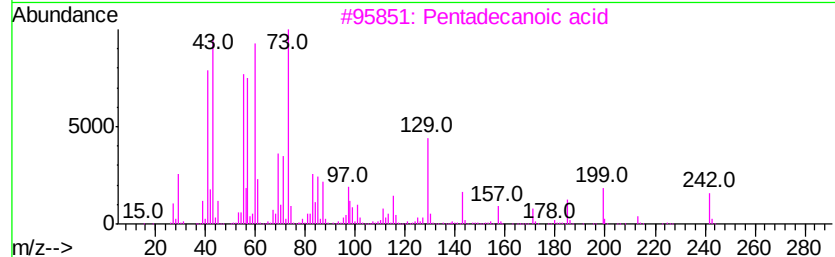
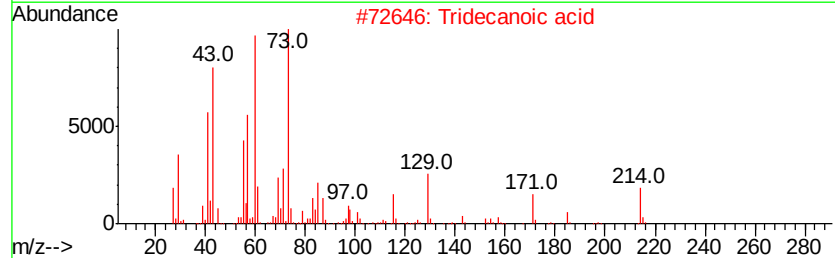
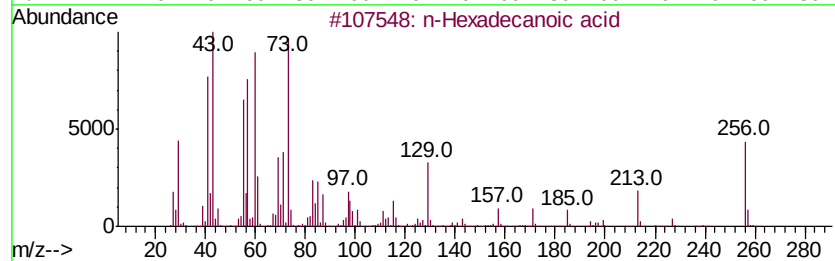
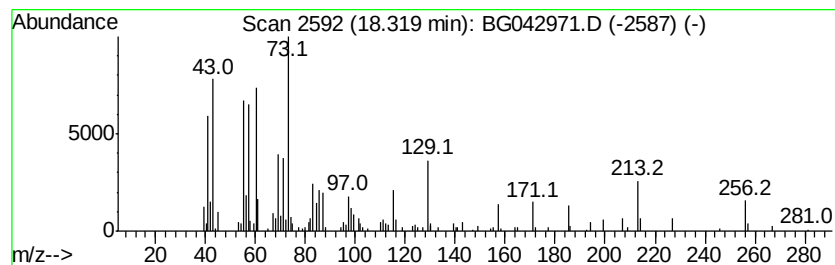
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.32	2.63 ng	150038	Phenanthrene-d10		17.43
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	50



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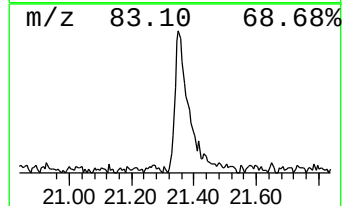
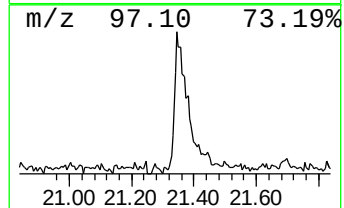
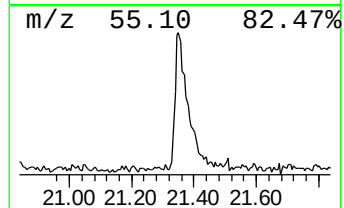
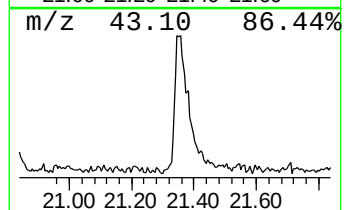
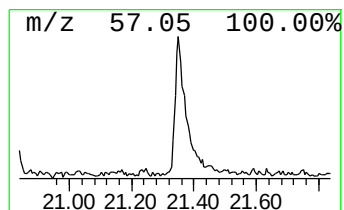
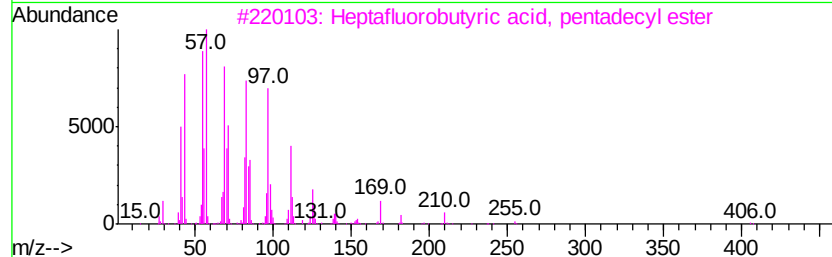
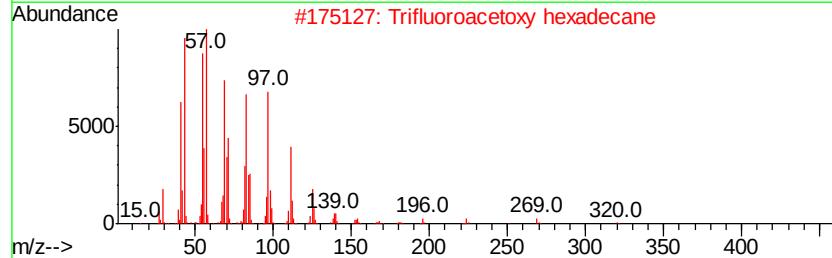
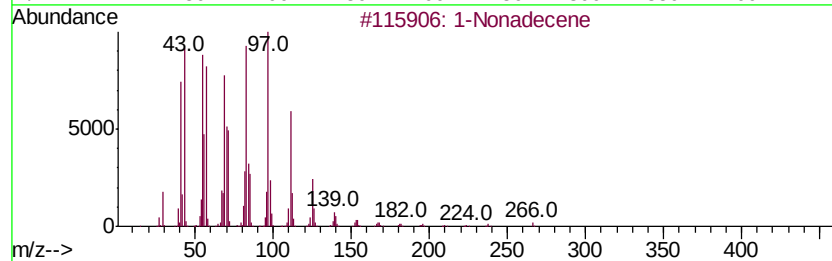
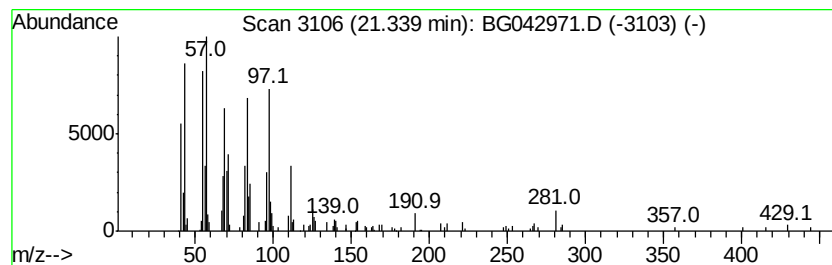
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Peak Number 6 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.34	5.10 ng	360089	Chrysene-d12	21.70		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	97
2	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	93
3	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	91
4	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	91
5	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pentene, 2-methyl-	3.18	10.3	ng	225373	1	8.07	438978	20.0
Butane, 2-methoxy...	3.26	5.5	ng	120510	1	8.07	438978	20.0
unknown7.61	7.61	71.0	ng	1559420	1	8.07	438978	20.0
n-Hexadecanoic acid	18.32	2.6	ng	150038	4	17.43	1142120	20.0
1-Nonadecene	21.34	5.1	ng	360089	5	21.70	1411410	20.0