

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
 Data File : BG042974.D
 Acq On : 1 Oct 2019 19:38
 Operator : JU
 Sample : K5079-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-1-COMP

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	3.177	8	15	25	rBV	587184	1366819	25.03%	4.616%
2	3.260	25	29	39	rVB	92487	160641	2.94%	0.543%
3	5.657	430	437	448	rBV	1112459	1877587	34.38%	6.342%
4	7.243	698	707	725	rBV	1243790	2194069	40.18%	7.410%
5	7.608	762	769	781	rBV	1181715	2057307	37.68%	6.949%
6	8.072	841	848	857	rBV	256819	441704	8.09%	1.492%
7	8.395	895	903	911	rBV	907803	1575168	28.85%	5.320%
8	9.229	1037	1045	1058	rBV	694555	1287717	23.58%	4.349%
9	10.874	1317	1325	1333	rBV	316010	584780	10.71%	1.975%
10	13.313	1733	1740	1752	rBV	1972413	3180850	58.25%	10.743%
11	14.135	1874	1880	1888	rBV	178551	271672	4.98%	0.918%
12	14.687	1967	1974	1982	rBV2	554647	877966	16.08%	2.965%
13	16.174	2220	2227	2238	rBV	1865615	2871603	52.59%	9.699%
14	17.431	2433	2441	2453	rBV	732770	1149839	21.06%	3.884%
15	18.318	2587	2592	2599	rBV2	121248	174700	3.20%	0.590%
16	20.040	2879	2885	2894	rBV	4220896	5460643	100.00%	18.443%
17	21.350	3103	3108	3121	rBV2	156648	398133	7.29%	1.345%
18	21.591	3145	3149	3155	rBV	55954	84942	1.56%	0.287%
19	21.697	3161	3167	3182	rVB	823997	1449172	26.54%	4.895%
20	22.514	3301	3306	3310	rBV2	49165	83323	1.53%	0.281%
21	23.207	3420	3424	3433	rVB3	64512	114518	2.10%	0.387%
22	23.401	3452	3457	3463	rVB3	43328	84251	1.54%	0.285%
23	24.018	3557	3562	3570	rVB2	71053	140824	2.58%	0.476%
24	24.923	3707	3716	3733	rVB2	488002	1572613	28.80%	5.311%
25	26.103	3912	3917	3929	rVB4	51054	146881	2.69%	0.496%

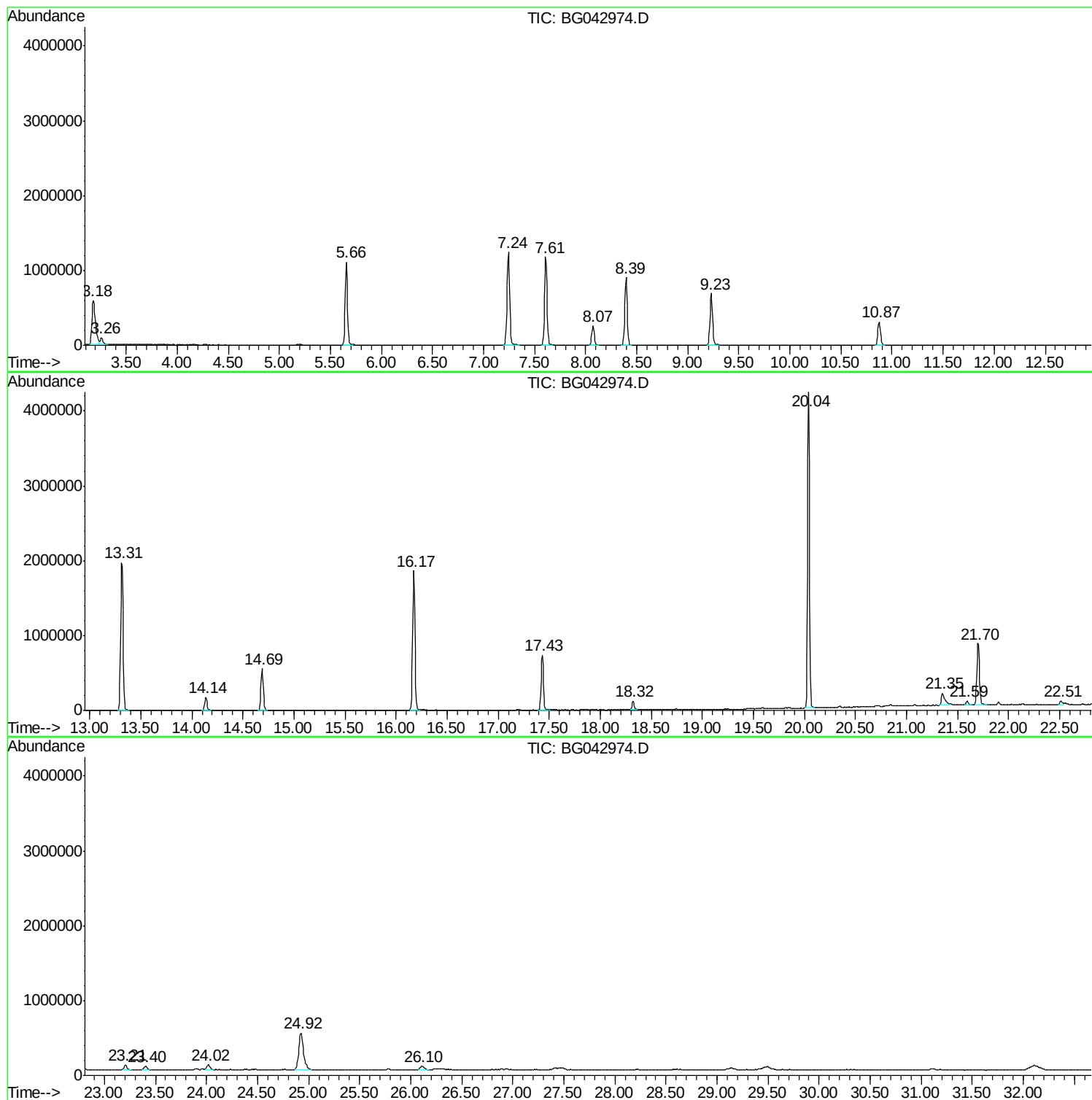
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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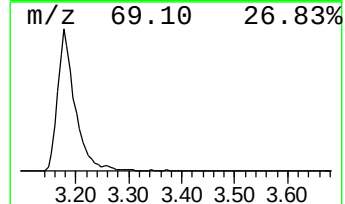
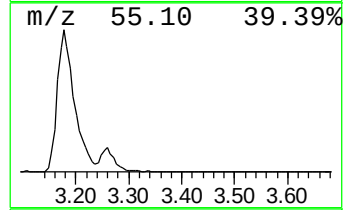
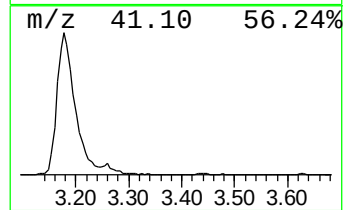
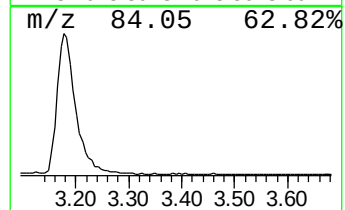
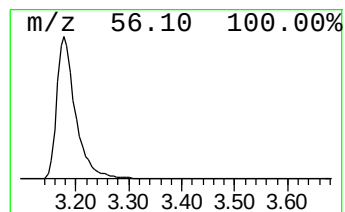
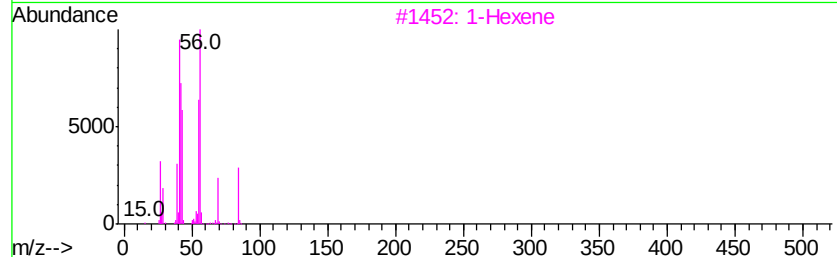
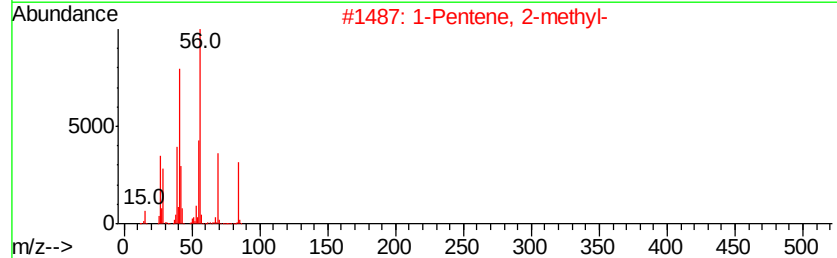
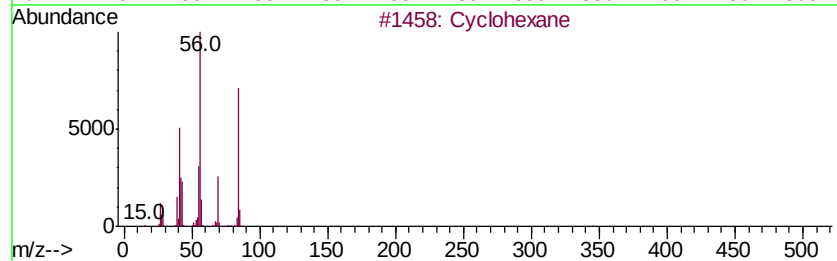
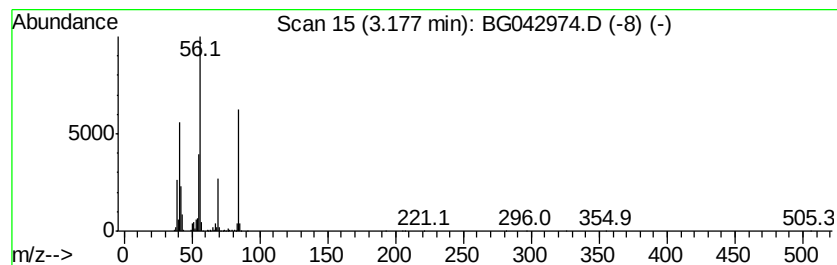
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	61.89 ng	1366820	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	72
3		1-Hexene	84	C6H12	000592-41-6	53
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	47
5		Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	45



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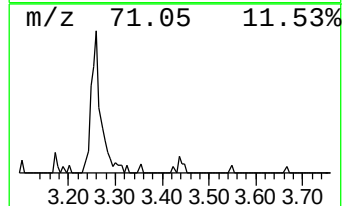
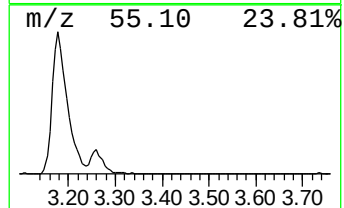
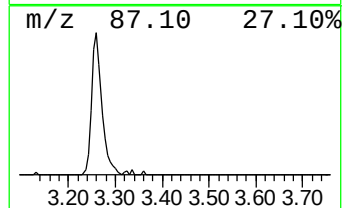
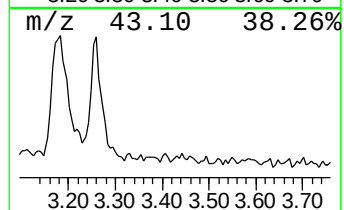
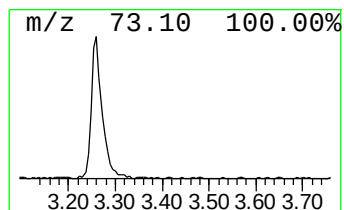
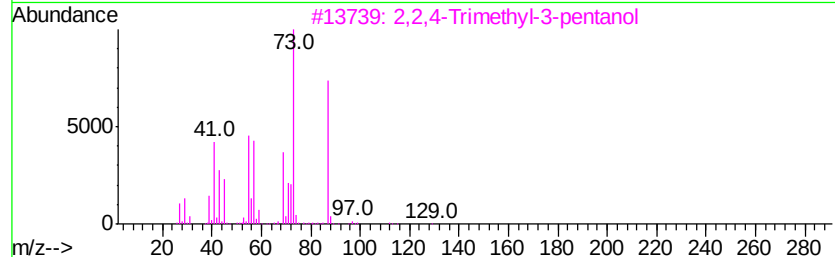
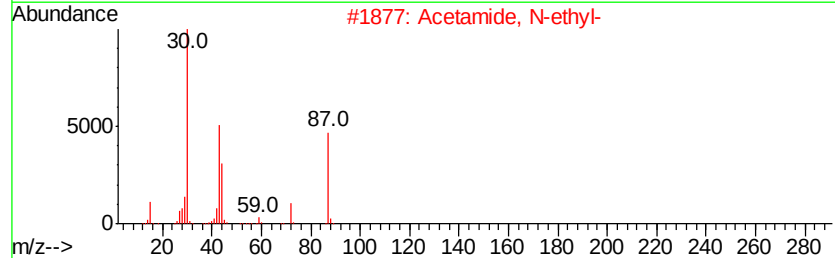
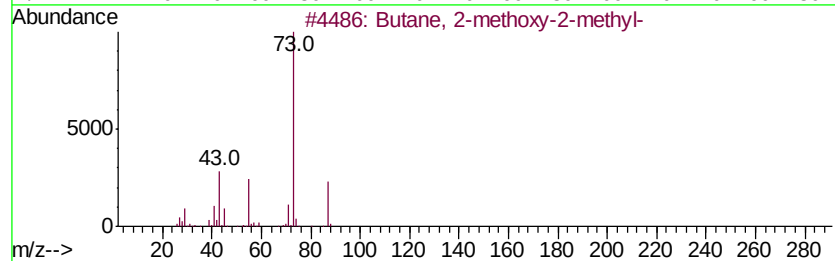
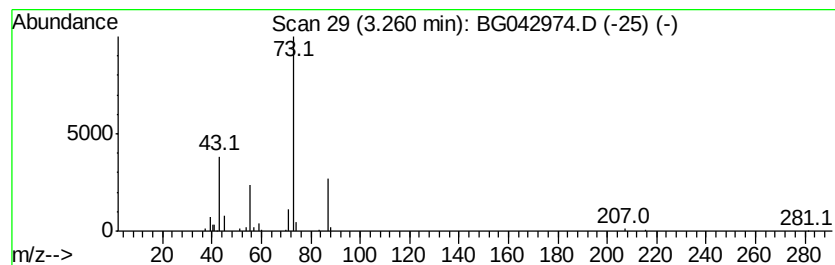
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	7.27 ng	160641	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	78
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	7



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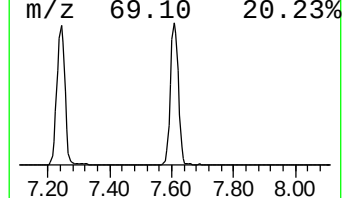
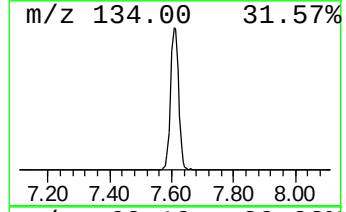
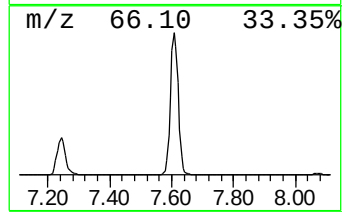
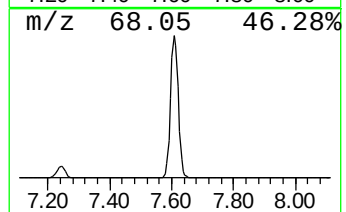
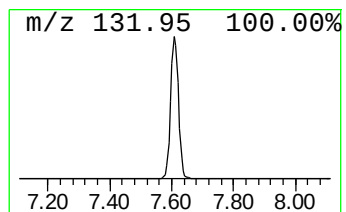
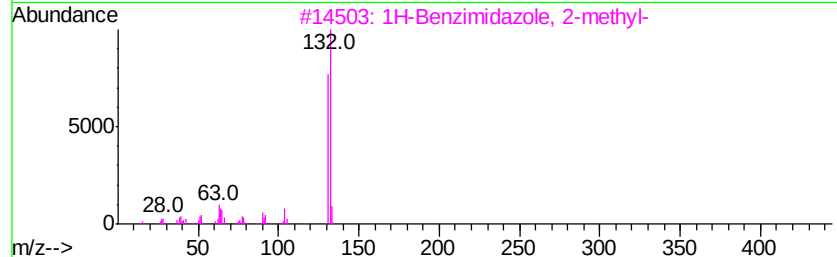
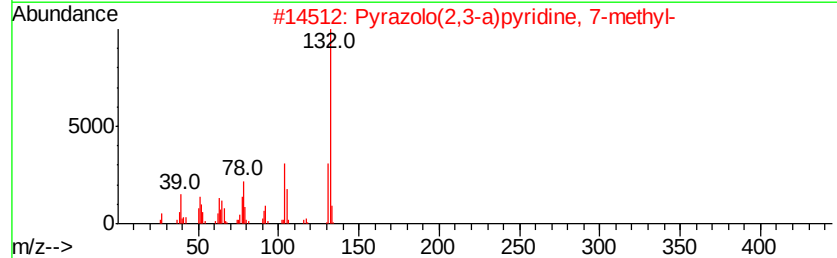
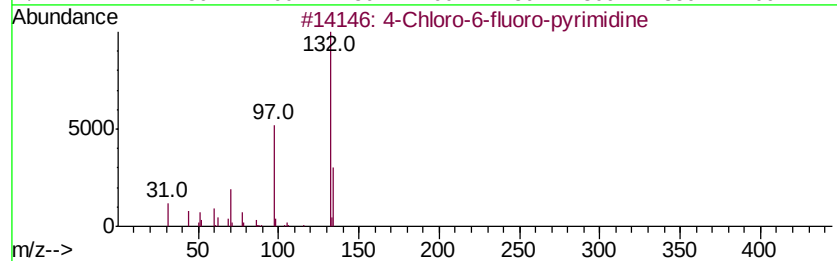
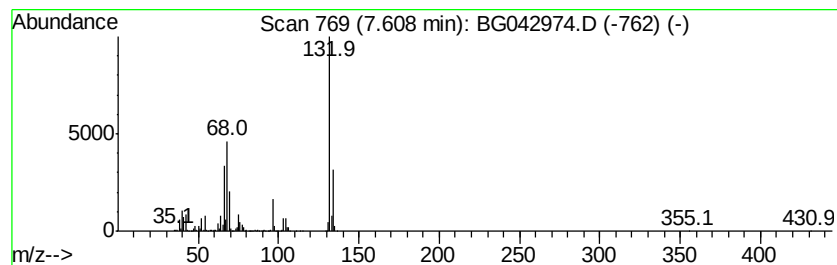
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	93.15 ng	2057310	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		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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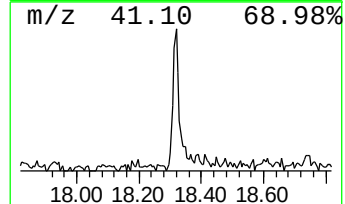
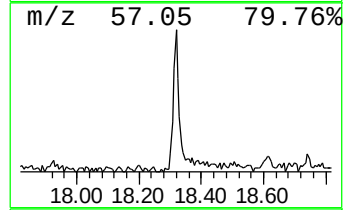
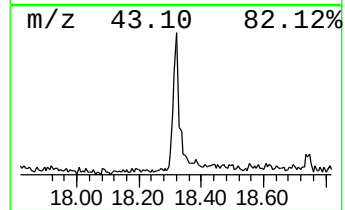
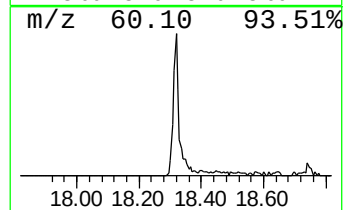
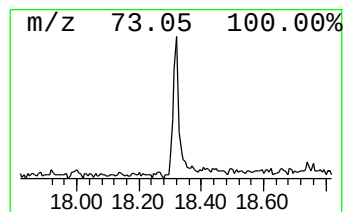
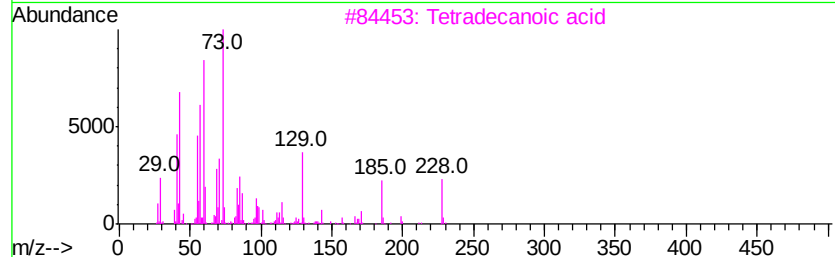
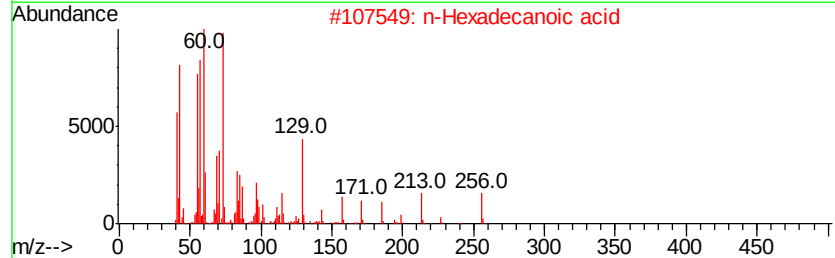
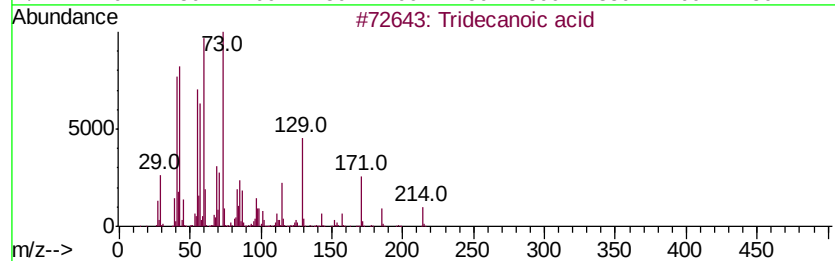
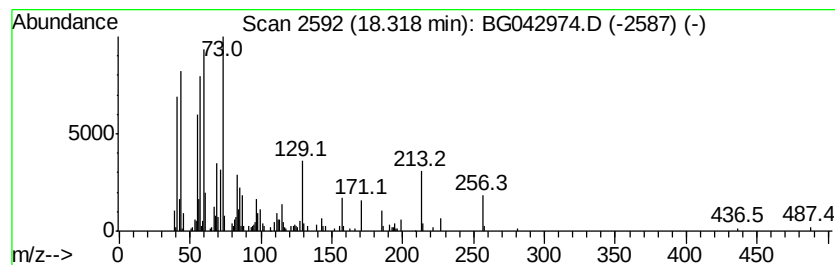
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Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	3.04 ng	174700	Phenanthrene-d10	17.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	72



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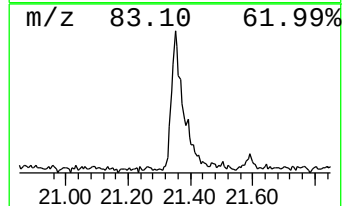
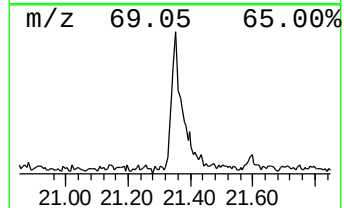
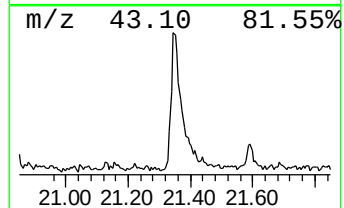
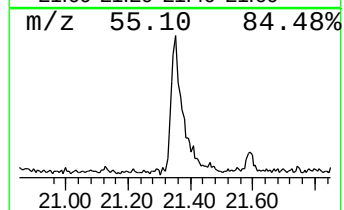
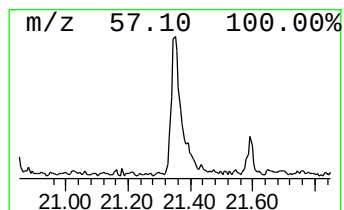
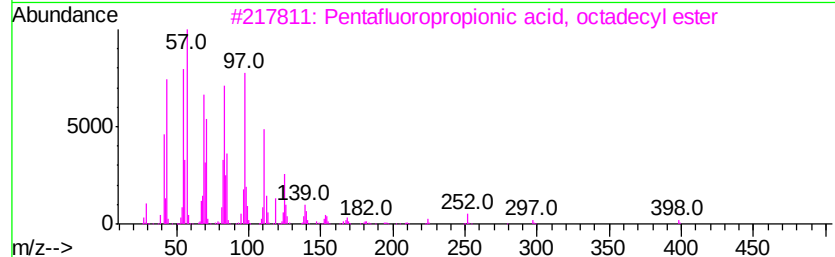
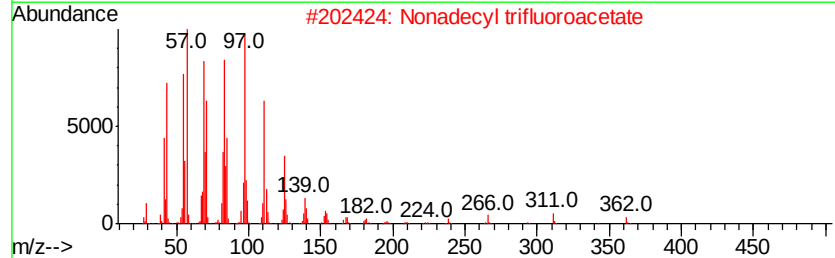
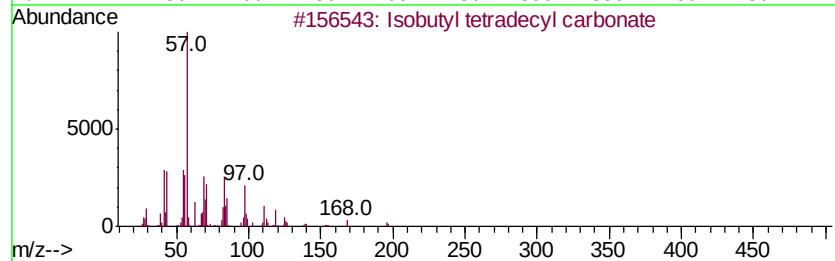
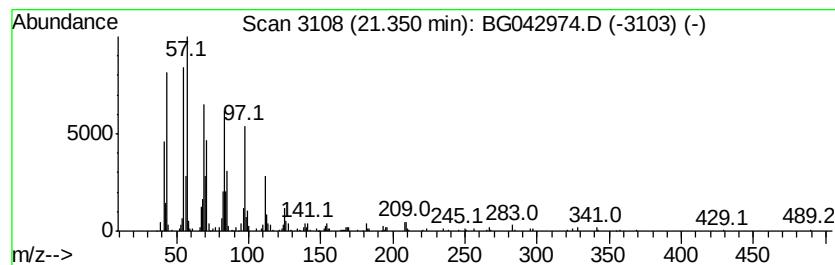
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Peak Number 6 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	5.49 ng	398133	Chrysene-d12	21.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
2		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5		1-Tricosene	322	C23H46	018835-32-0	90



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pentene, 2-methyl-	3.18	61.9	ng	1366820	1	8.07	441704	20.0
Butane, 2-methoxy...	3.26	7.3	ng	160641	1	8.07	441704	20.0
unknown7.61	7.61	93.2	ng	2057310	1	8.07	441704	20.0
Tridecanoic acid	18.32	3.0	ng	174700	4	17.43	1149840	20.0
Isobutyl tetradec...	21.35	5.5	ng	398133	5	21.70	1449170	20.0