

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG061818\
 Data File : BG035246.D
 Acq On : 19 Jun 2018 10:05
 Operator : SJ/JU
 Sample : J3566-16
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-6-S

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

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	3.980	114	118	128	rVB	49736	77903	1.13%	0.358%
2	4.579	214	220	235	rVB	258717	428899	6.22%	1.974%
3	5.636	393	400	412	rBV	817891	1359674	19.71%	6.257%
4	7.217	659	669	680	rBV	783211	1427906	20.70%	6.571%
5	7.593	725	733	743	rBV	884790	1529861	22.18%	7.040%
6	8.062	806	813	822	rVB2	151760	262965	3.81%	1.210%
7	8.386	860	868	875	rBV	593559	1061194	15.39%	4.883%
8	9.220	1002	1010	1020	rVB	544932	1004343	14.56%	4.621%
9	10.865	1283	1290	1296	rBV	174078	318103	4.61%	1.464%
10	13.308	1699	1706	1716	rBV	1487731	2307889	33.46%	10.620%
11	14.683	1931	1940	1947	rBV2	280644	459339	6.66%	2.114%
12	16.169	2185	2193	2208	rBV	1533395	2425994	35.17%	11.163%
13	17.426	2398	2407	2418	rBV2	496660	799445	11.59%	3.679%
14	18.302	2552	2556	2563	rBV3	59338	89551	1.30%	0.412%
15	20.035	2844	2851	2858	rBV	5142758	6897263	100.00%	31.738%
16	21.691	3126	3133	3145	rBV	561005	942338	13.66%	4.336%
17	24.916	3673	3682	3695	rBV4	92054	339321	4.92%	1.561%

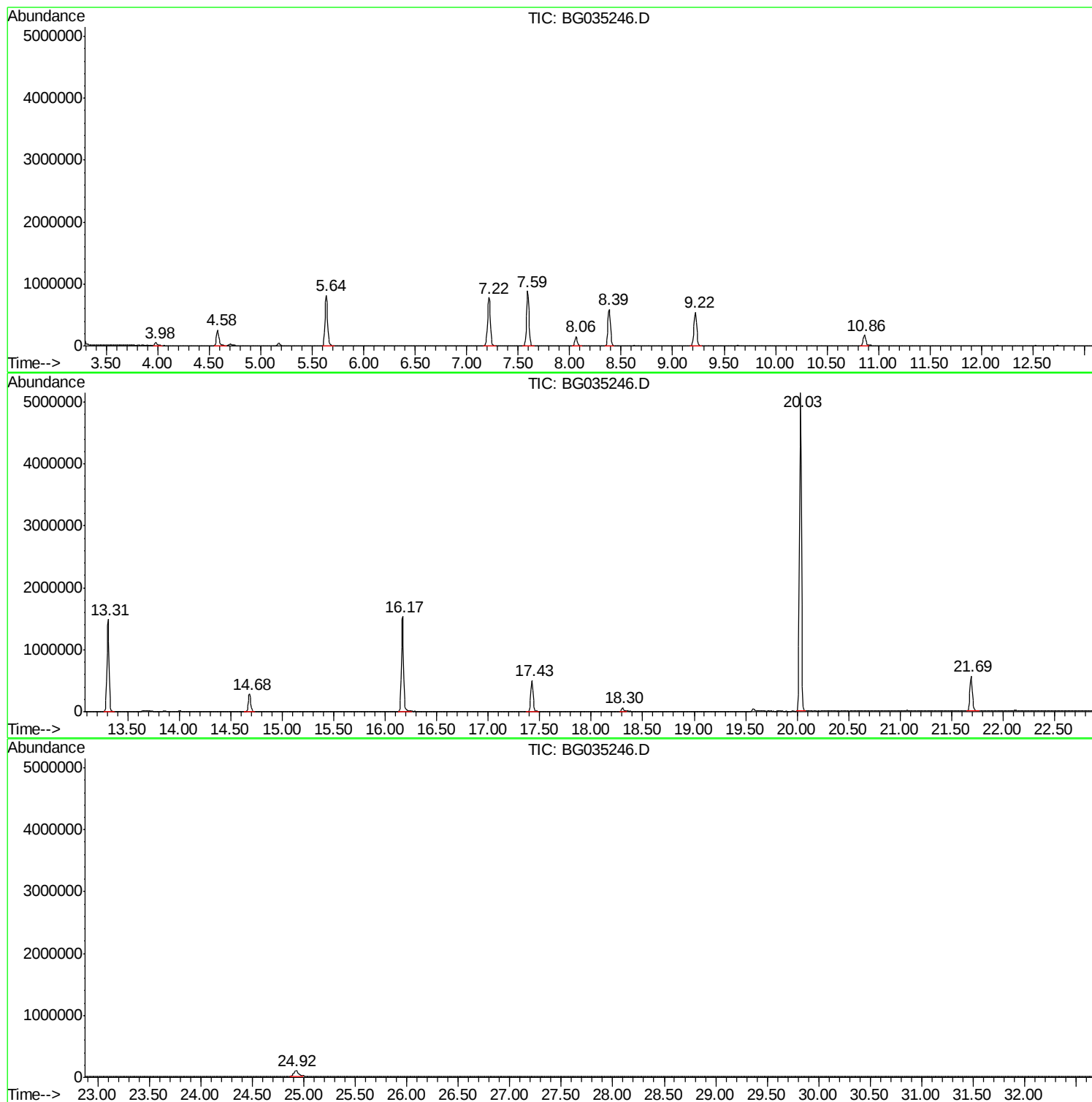
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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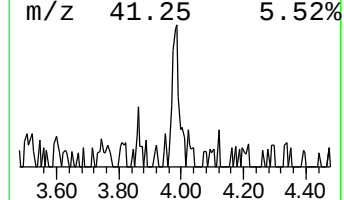
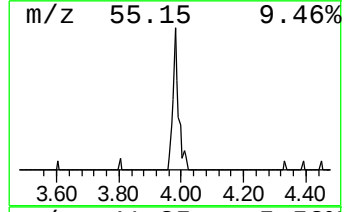
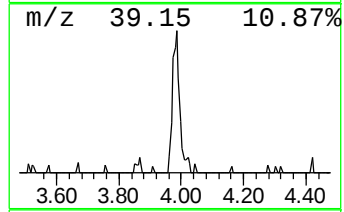
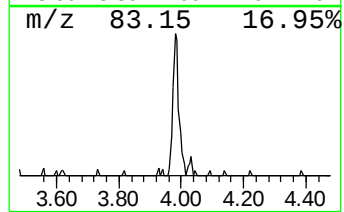
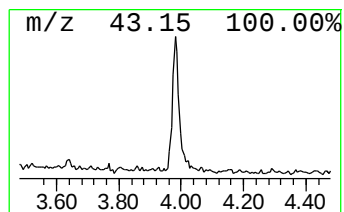
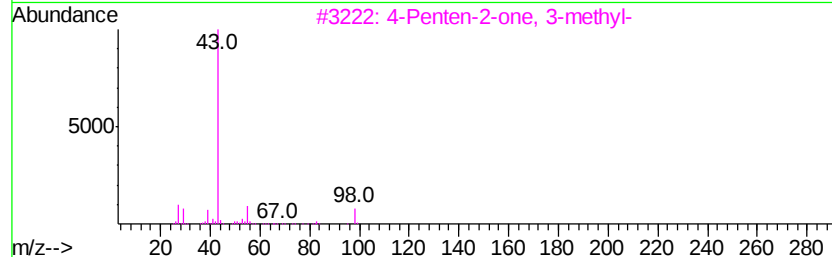
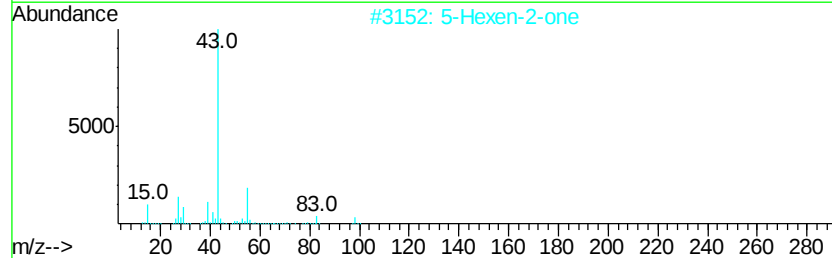
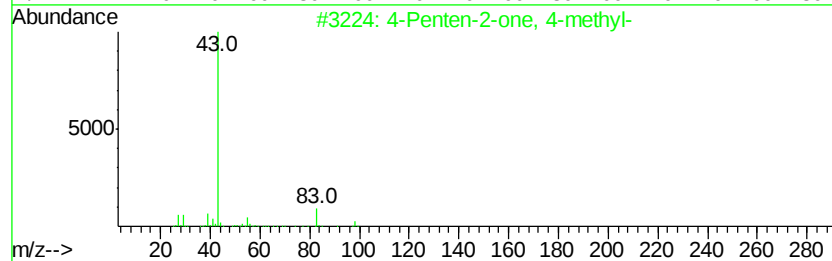
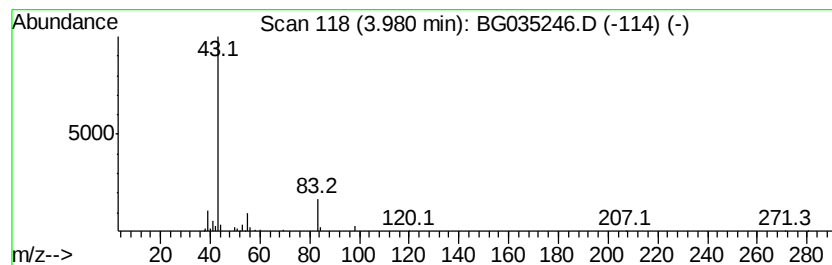
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	5.92 ng	77903	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	52
2			5-Hexen-2-one	98	C6H10O	000109-49-9	50
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
4			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	10
5			2H-Pyran, 3,4-dihydro-6-methyl-	98	C6H10O	016015-11-5	9



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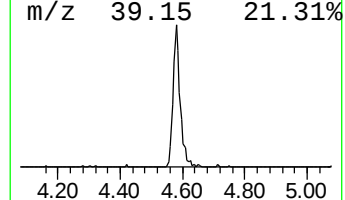
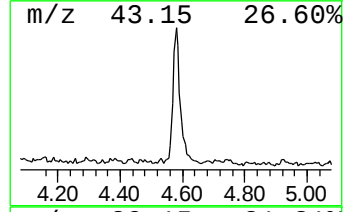
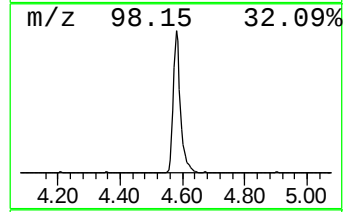
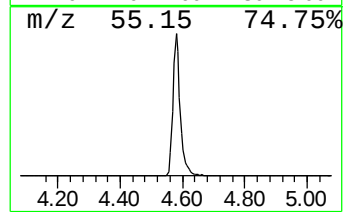
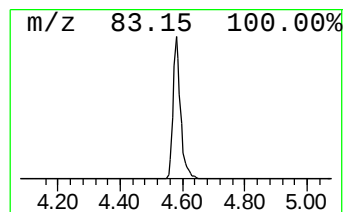
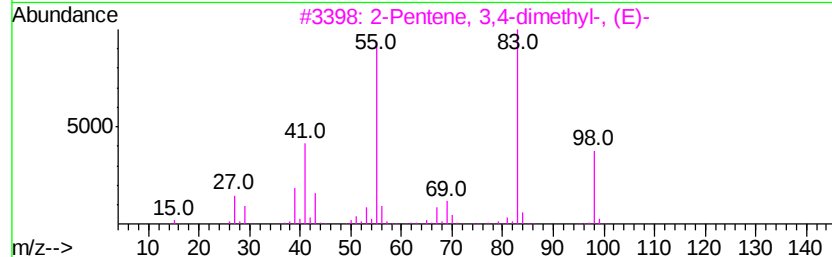
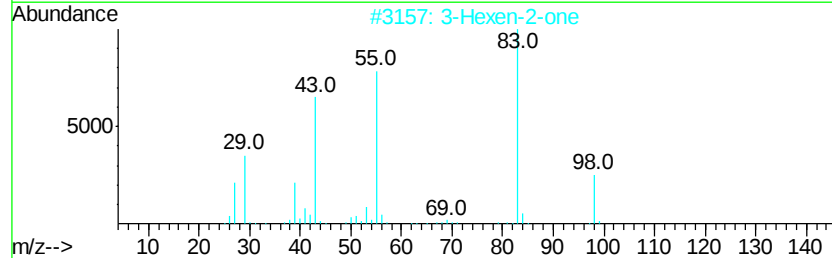
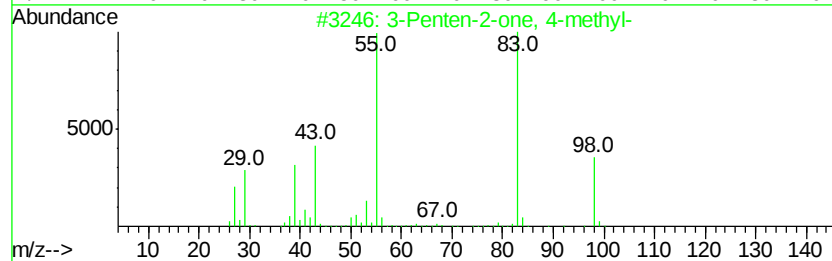
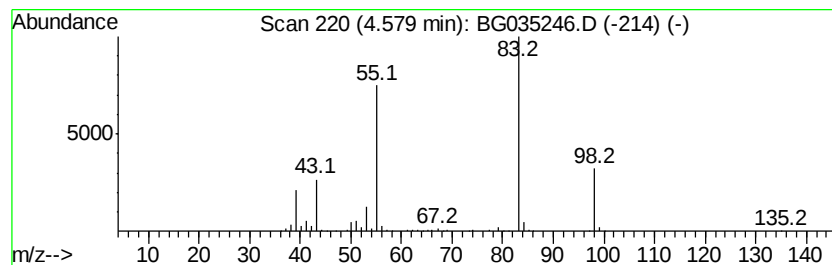
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	32.62 ng	428899	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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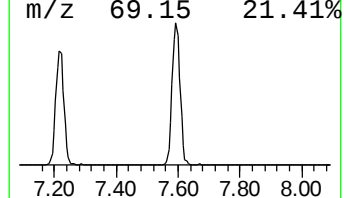
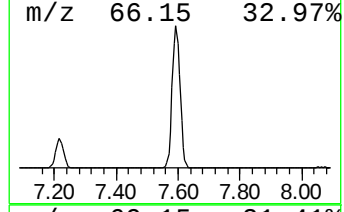
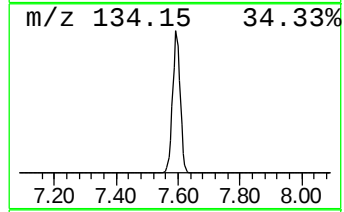
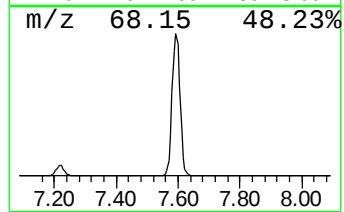
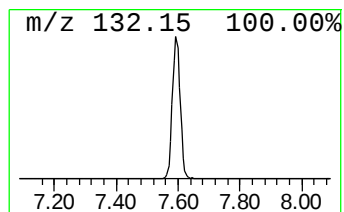
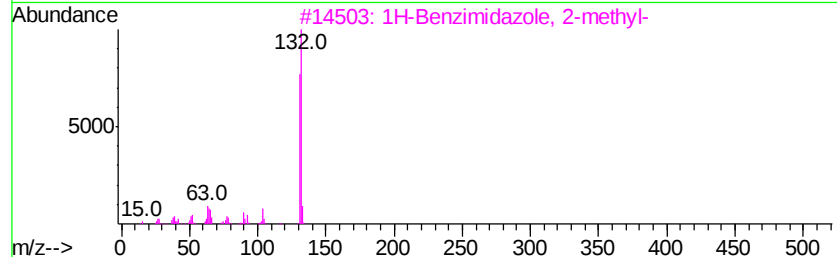
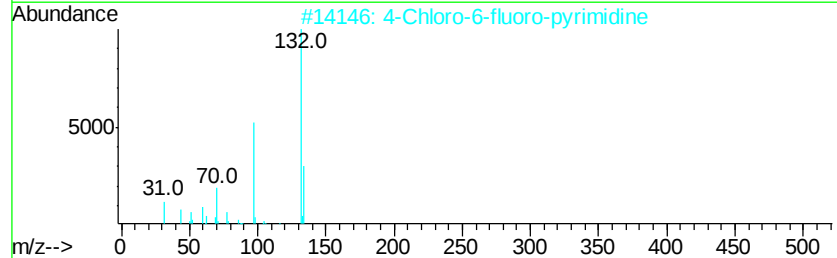
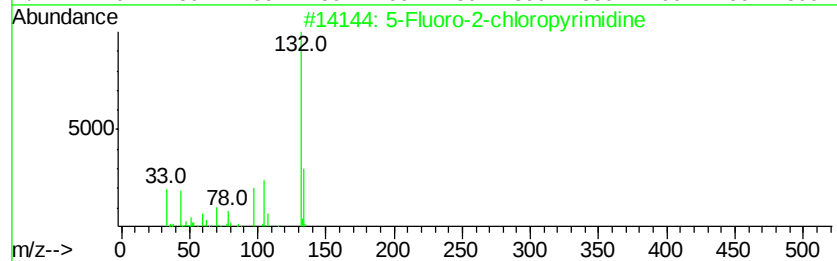
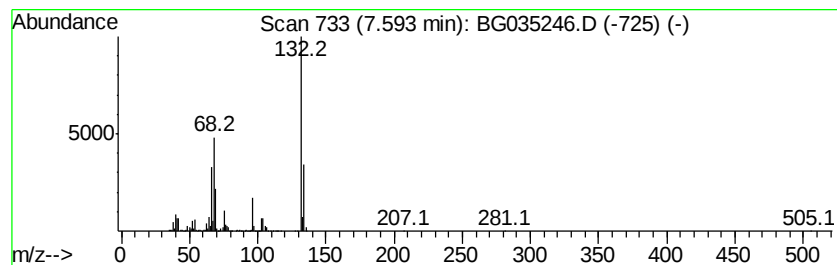
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Peak Number 3 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	116.36 ng	1529860	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	16



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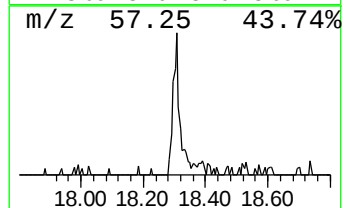
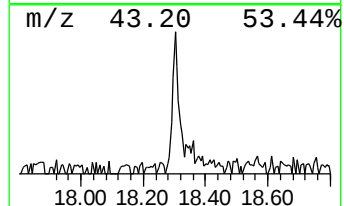
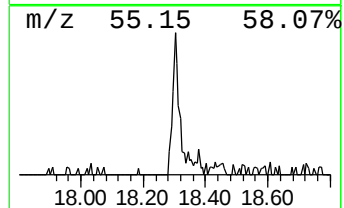
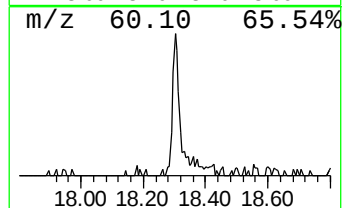
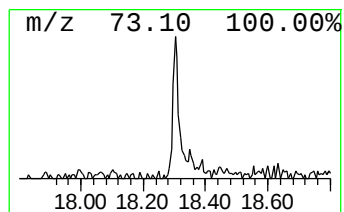
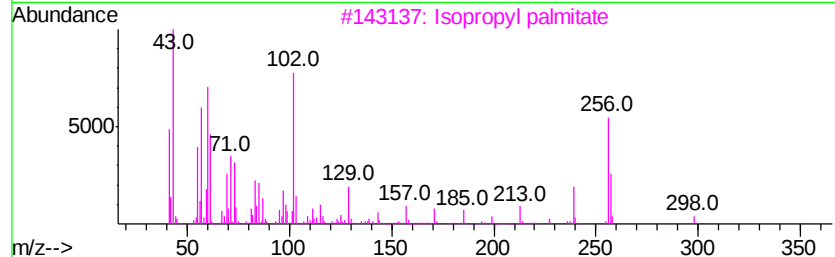
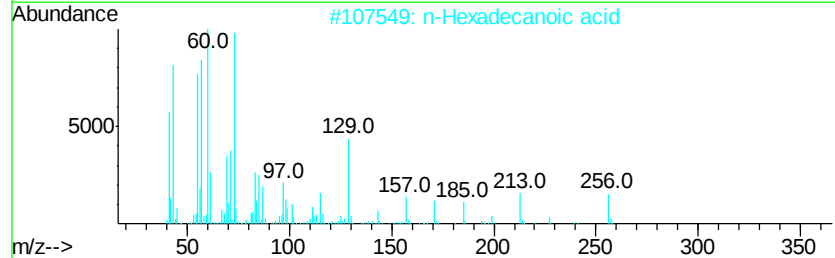
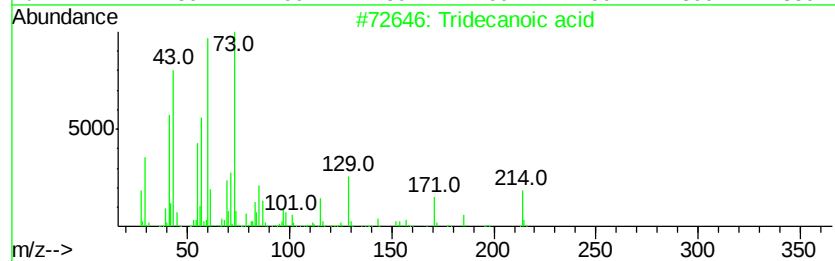
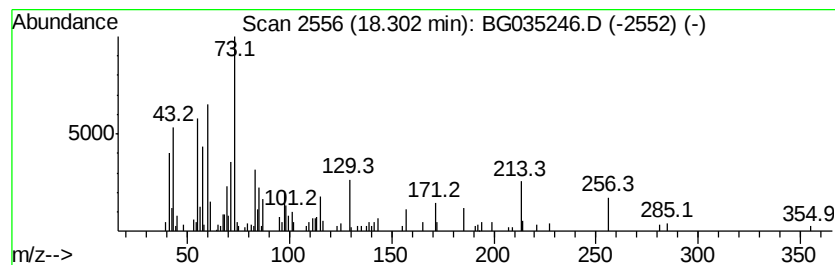
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Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.24 ng	89551	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3	Isopropyl palmitate	298	C19H38O2	000142-91-6	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.98	5.9	ng	77903	1	8.06	262965	20.0
3-Penten-2-one, 4...	4.58	32.6	ng	428899	1	8.06	262965	20.0
unknown7.59	7.59	116.4	ng	1529860	1	8.06	262965	20.0
Tridecanoic acid	18.30	2.2	ng	89551	4	17.42	799445	20.0