

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
 Data File : BG022276.D
 Acq On : 10 Jun 2016 2:31
 Operator : UM/SJ
 Sample : H3396-01
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 STA-928-PLATFORM(0-4)

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:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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	4.577	289	296	309	rBV	234312	410155	17.61%	3.291%
2	5.188	388	400	412	rBV	102197	195099	8.38%	1.565%
3	5.670	474	482	496	rBV	421214	793226	34.06%	6.365%
4	7.280	748	756	769	rBV	437279	861106	36.97%	6.909%
5	7.650	810	819	831	rBV	531106	1027600	44.12%	8.245%
6	8.114	885	898	908	rBV	95792	191941	8.24%	1.540%
7	8.443	945	954	974	rBV	414285	811881	34.86%	6.514%
8	9.289	1090	1098	1119	rBV	300112	622840	26.74%	4.998%
9	10.940	1368	1379	1386	rBV	157635	336766	14.46%	2.702%
10	13.367	1784	1792	1802	rBV	1030654	1827167	78.45%	14.661%
11	14.748	2020	2027	2035	rBV2	265632	469678	20.17%	3.769%
12	16.234	2272	2280	2292	rBV	635827	1107271	47.54%	8.885%
13	17.492	2486	2494	2506	rBV	294937	500826	21.50%	4.019%
14	19.759	2875	2880	2884	rBV	50636	65195	2.80%	0.523%
15	20.083	2929	2935	2949	rBV	1602019	2329149	100.00%	18.689%
16	20.794	3052	3056	3060	rBV	34679	43846	1.88%	0.352%
17	21.763	3214	3221	3234	rBV2	246033	501340	21.52%	4.023%
18	25.065	3771	3783	3797	rBV3	97456	367607	15.78%	2.950%

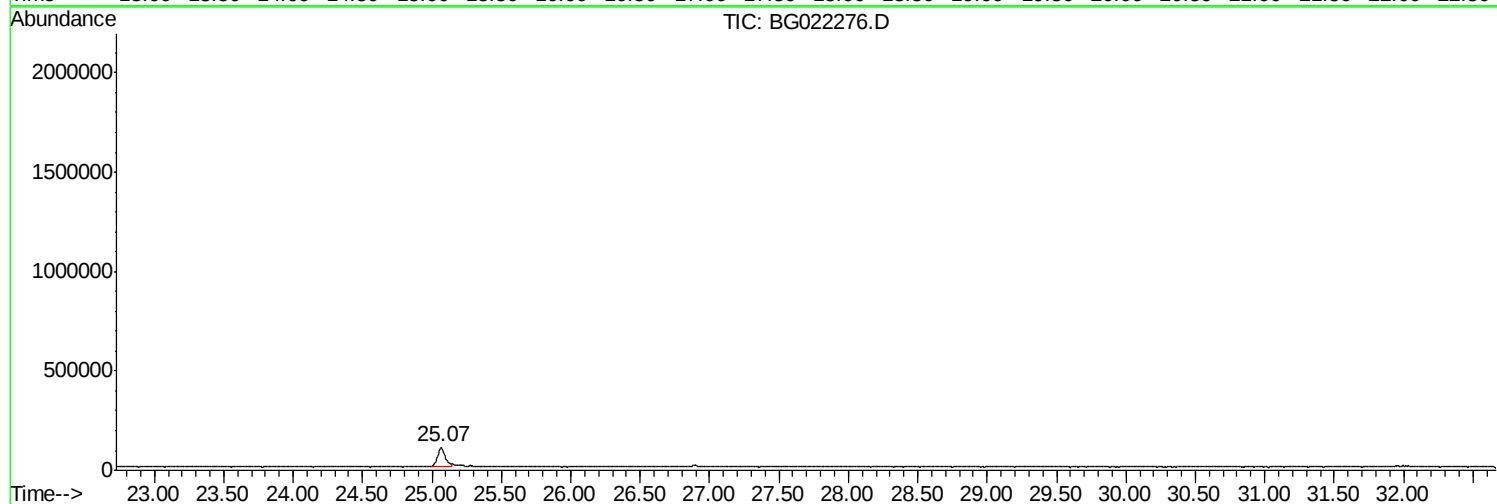
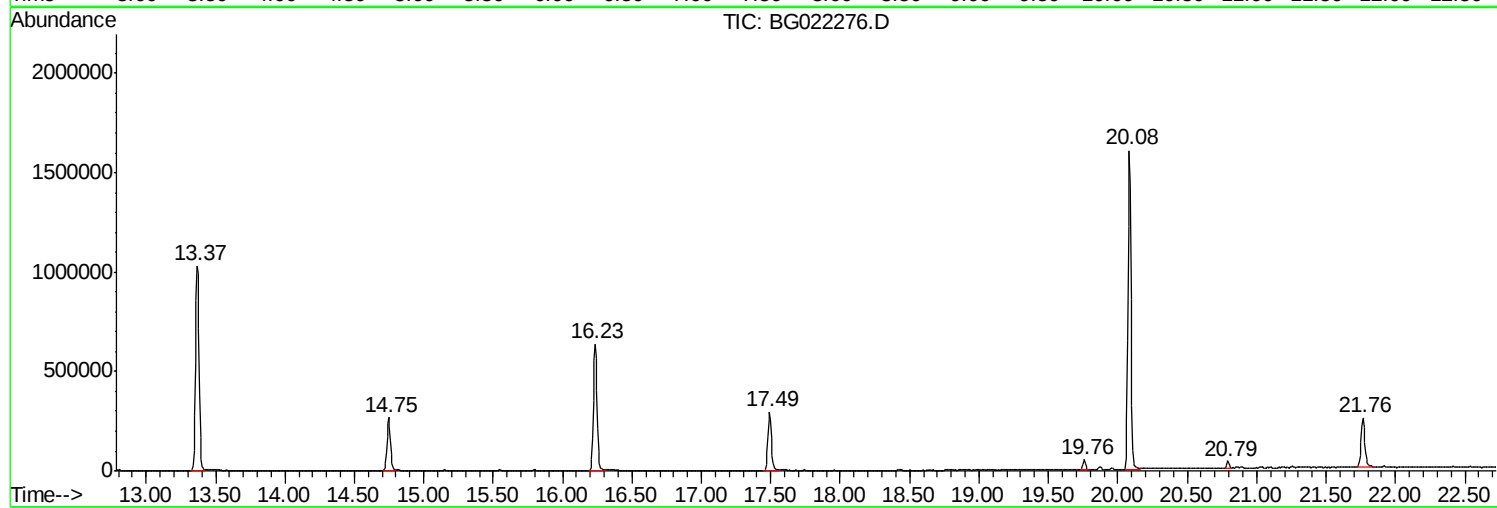
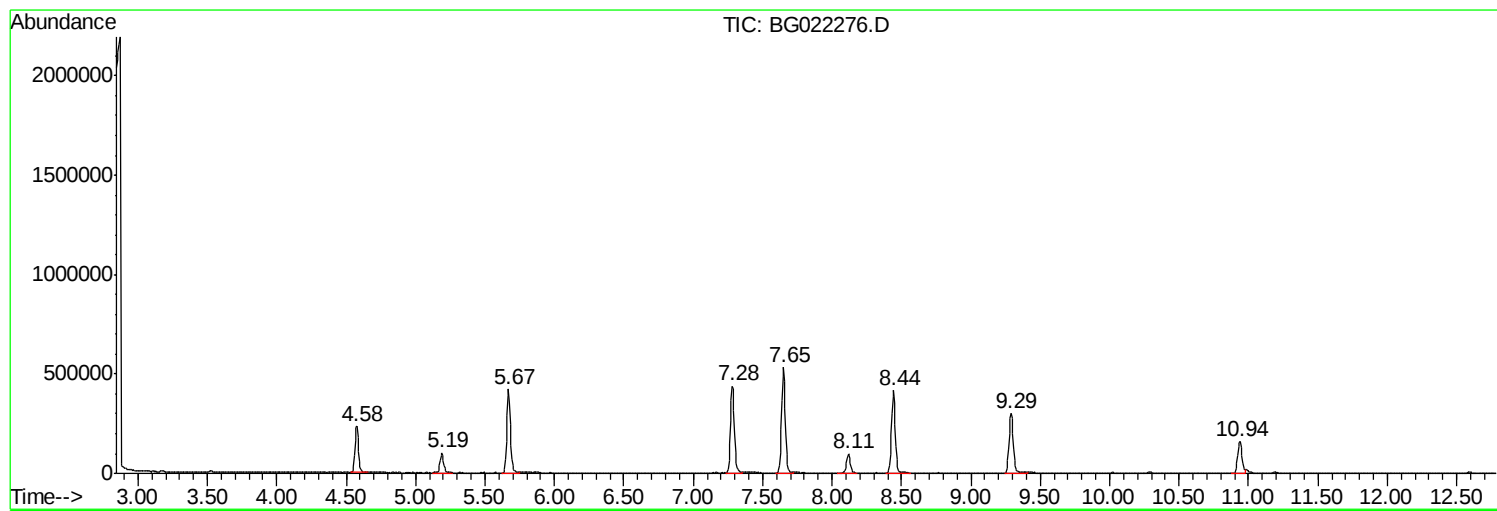
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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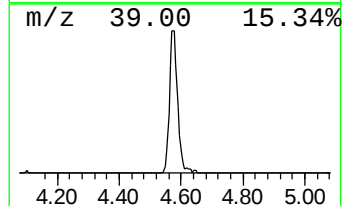
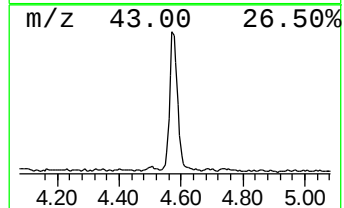
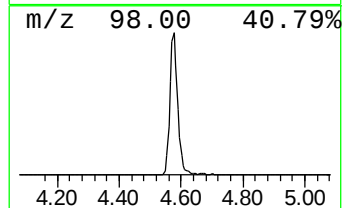
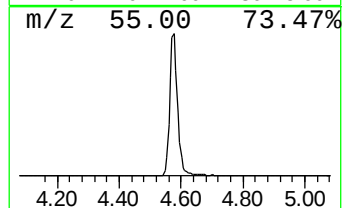
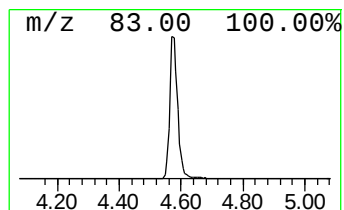
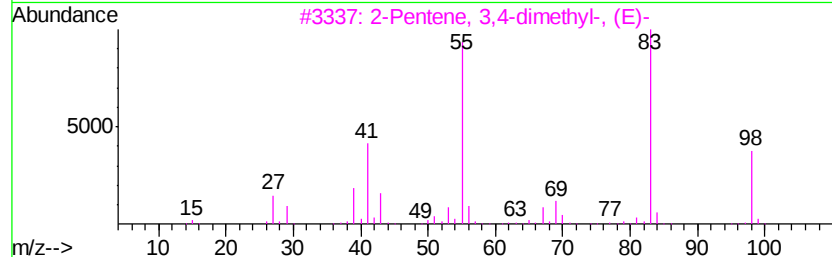
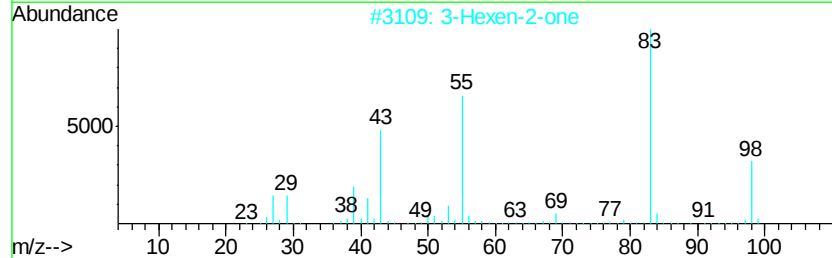
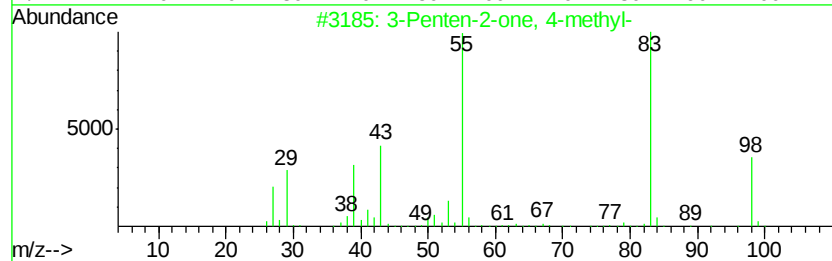
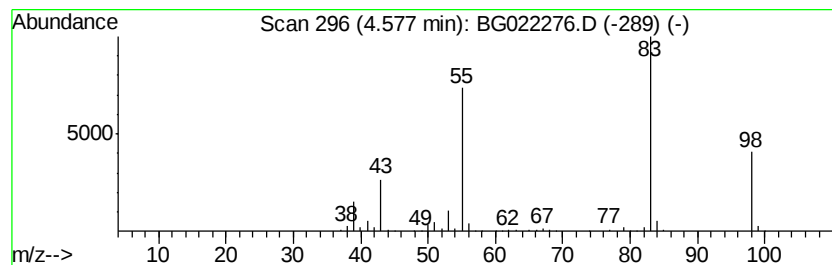
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	42.74 ng	410155	1,4-Dichlorobenzene-d4	8.11

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		Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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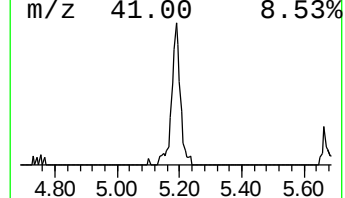
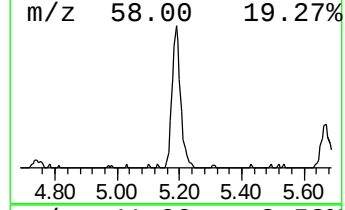
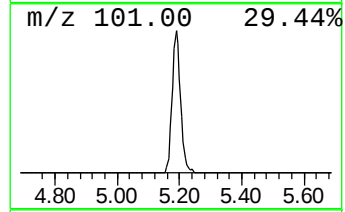
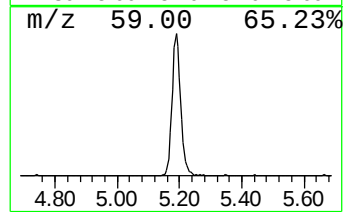
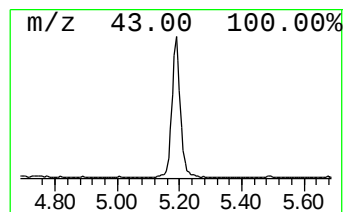
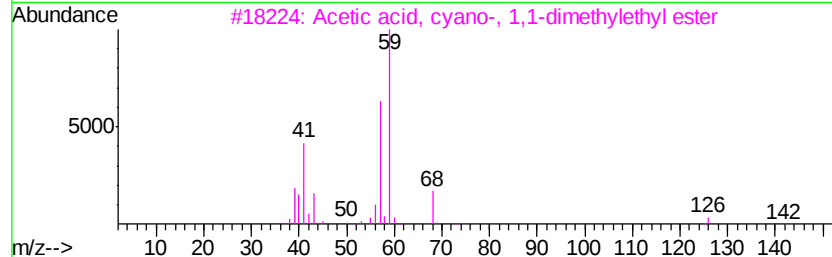
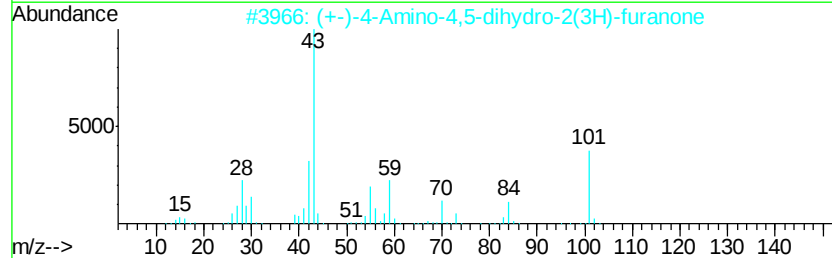
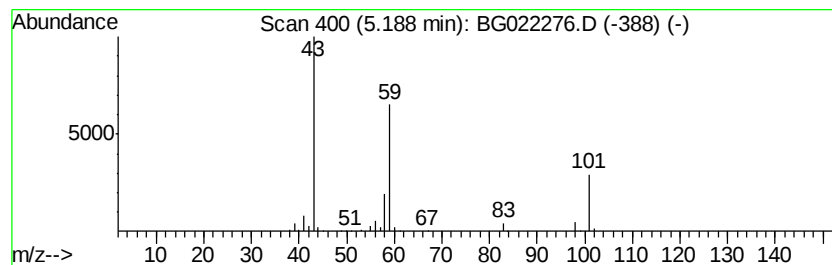
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	20.33 ng	195099	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	12
4		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	10
5		Guanidine	59	CH5N3	000113-00-8	9



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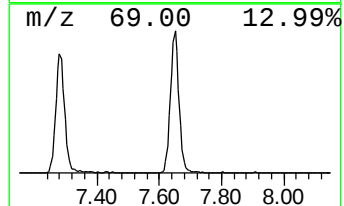
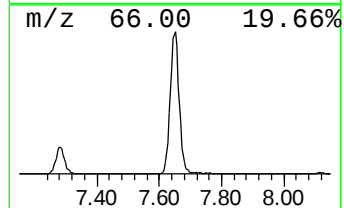
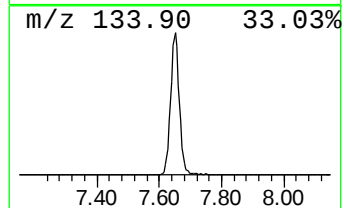
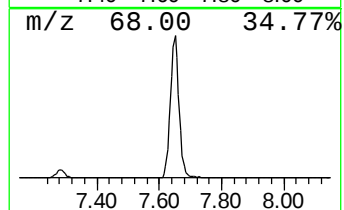
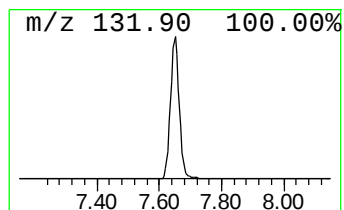
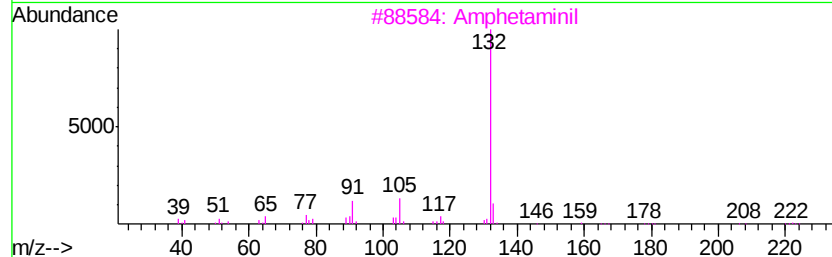
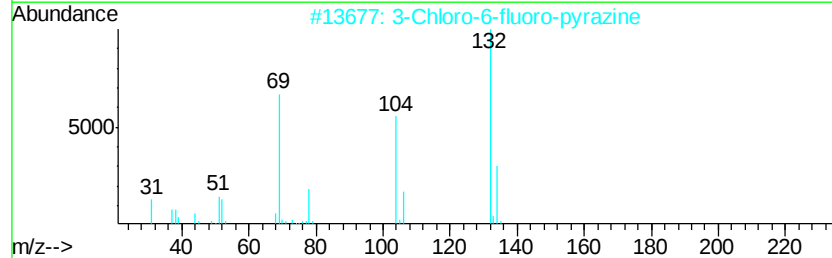
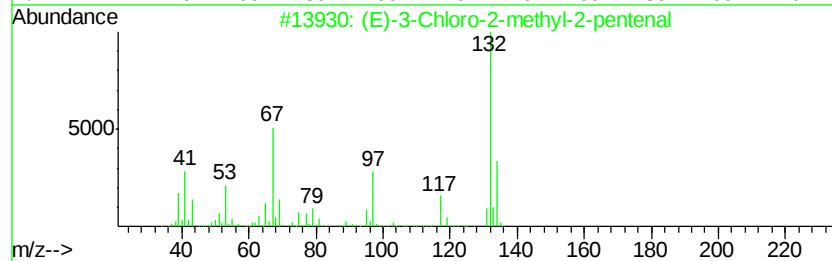
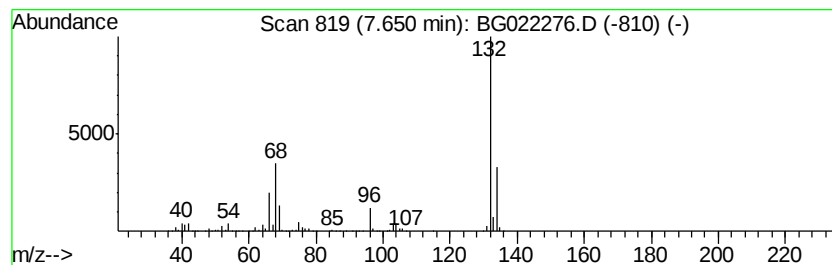
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Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	107.08 ng	1027600	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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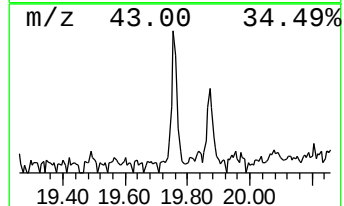
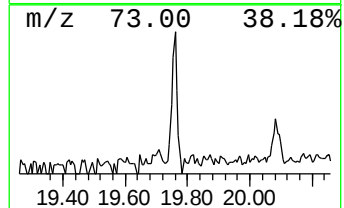
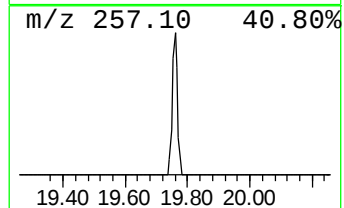
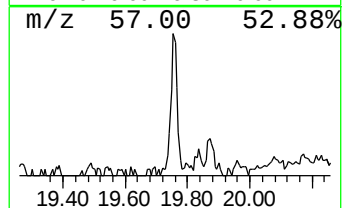
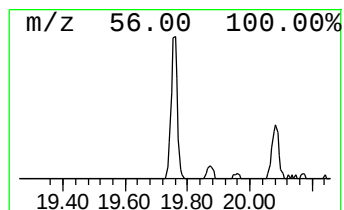
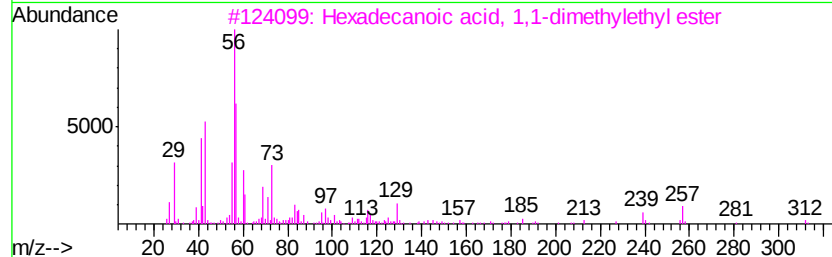
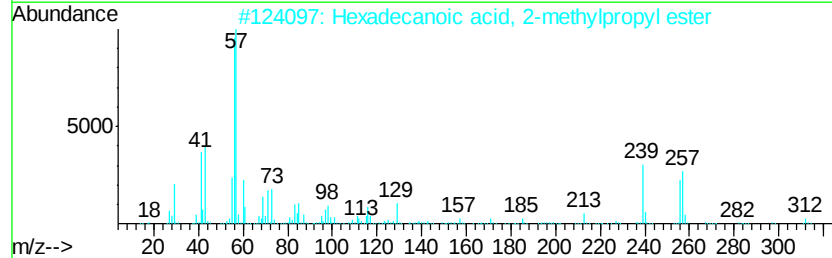
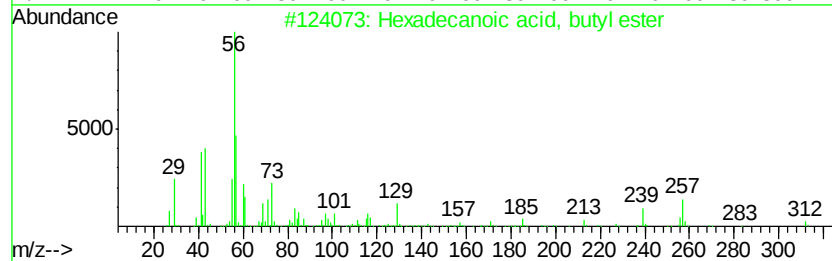
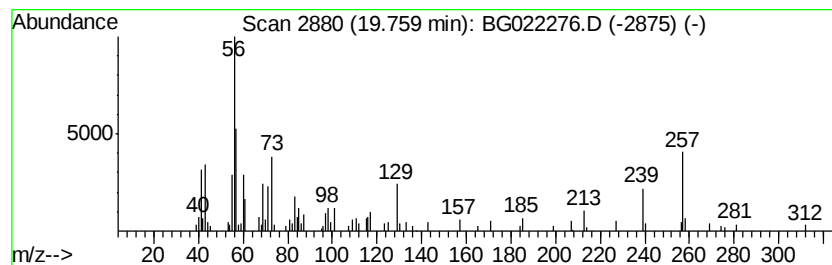
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.76	2.60 ng	65195	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	90
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
4		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.58	42.7	ng	410155	1	8.11	191941	20.0
2-Pentanone, 4-hy...	5.19	20.3	ng	195099	1	8.11	191941	20.0
unknown7.65	7.65	107.1	ng	1027600	1	8.11	191941	20.0
Hexadecanoic acid...	19.76	2.6	ng	65195	5	21.76	501340	20.0