

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112118\
 Data File : BG038120.D
 Acq On : 21 Nov 2018 16:57
 Operator : JU/SJ
 Sample : PB114976BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB114976BL

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-BG111318.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	5.168	313	320	326	rBV	35652	57511	2.17%	0.392%
2	5.632	390	399	409	rBV	667417	1135514	42.91%	7.738%
3	7.236	664	672	684	rBV	700890	1247410	47.13%	8.500%
4	7.612	728	736	748	rBV	667199	1182423	44.68%	8.057%
5	8.088	810	817	824	rBV	130627	232915	8.80%	1.587%
6	8.411	864	872	881	rVB	483801	883648	33.39%	6.021%
7	9.263	1008	1017	1026	rBV	422831	790506	29.87%	5.387%
8	10.902	1288	1296	1304	rBV	182645	352312	13.31%	2.401%
9	13.340	1704	1711	1720	rBV	1146156	1835820	69.37%	12.510%
10	14.721	1939	1946	1956	rVB2	309913	507814	19.19%	3.460%
11	16.208	2193	2199	2215	rBV2	677853	1130556	42.72%	7.704%
12	17.465	2407	2413	2423	rBV	403387	630811	23.84%	4.299%
13	19.733	2794	2799	2808	rBV	197137	233576	8.83%	1.592%
14	19.850	2815	2819	2827	rVB	43714	51673	1.95%	0.352%
15	20.068	2850	2856	2863	rBV	2015722	2646503	100.00%	18.034%
16	20.773	2972	2976	2982	rBV	155071	177099	6.69%	1.207%
17	21.748	3135	3142	3156	rBV	394681	686381	25.94%	4.677%
18	21.895	3162	3167	3172	rBV	27411	38004	1.44%	0.259%
19	22.512	3267	3272	3278	rVB2	26346	41817	1.58%	0.285%
20	23.223	3387	3393	3402	rVB3	29064	59938	2.26%	0.408%
21	24.040	3526	3532	3541	rVB4	25073	55574	2.10%	0.379%
22	25.074	3689	3708	3722	rBV2	184508	665157	25.13%	4.533%
23	27.571	4122	4133	4142	rVB7	10125	32086	1.21%	0.219%

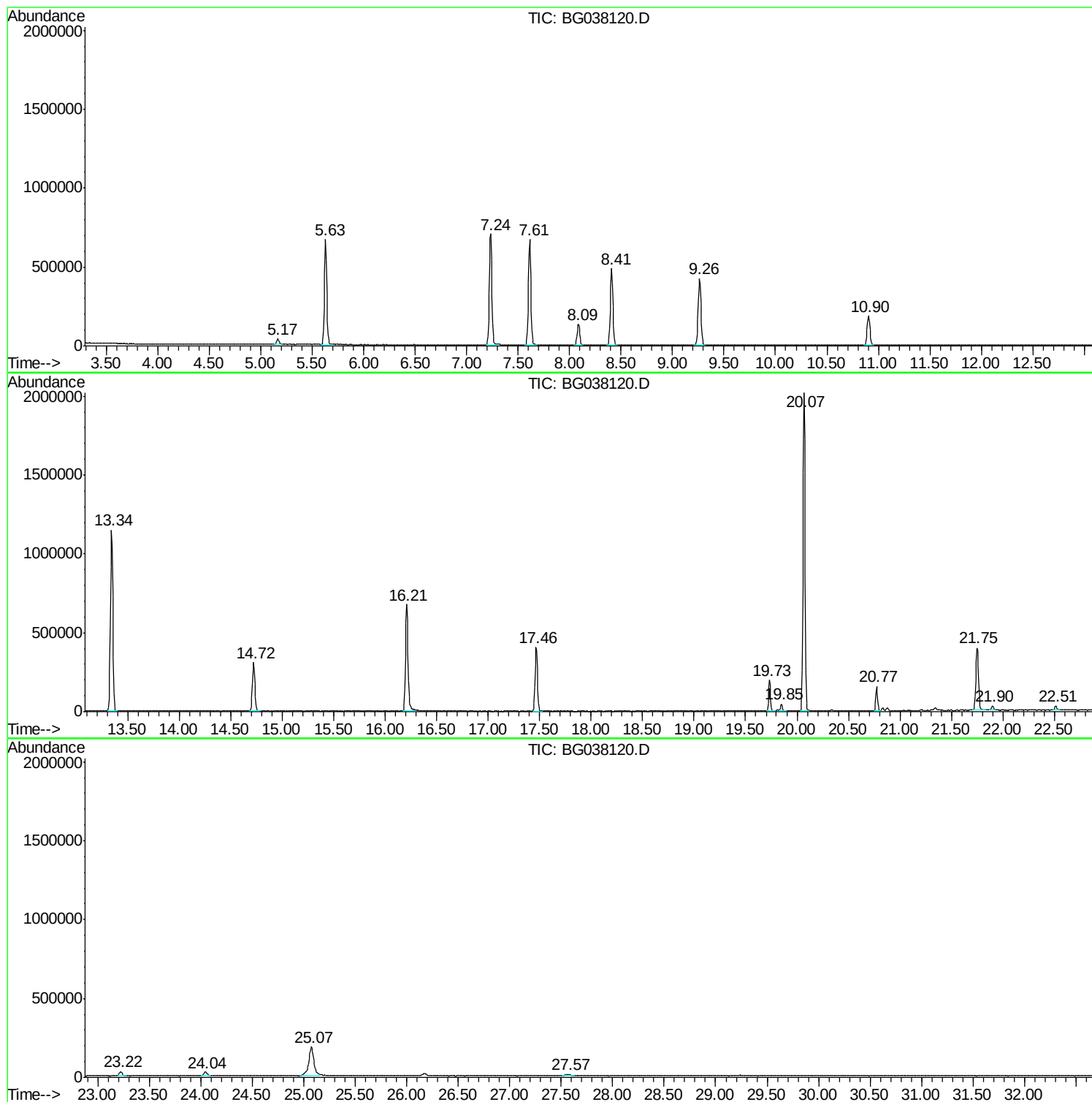
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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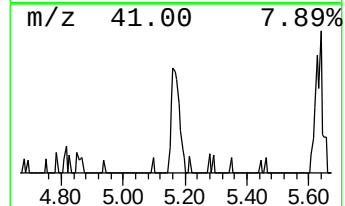
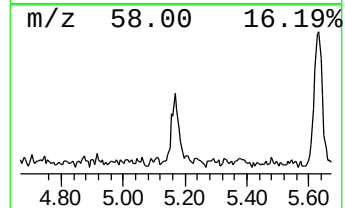
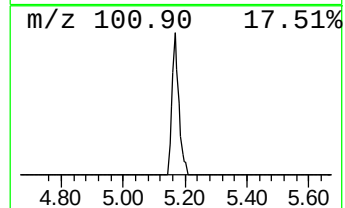
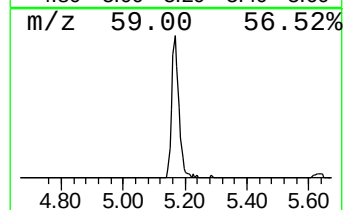
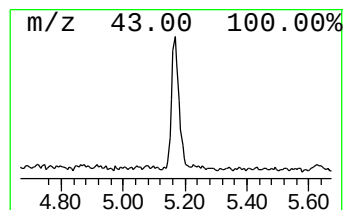
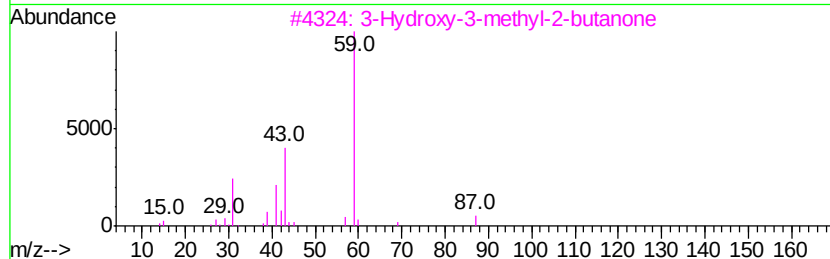
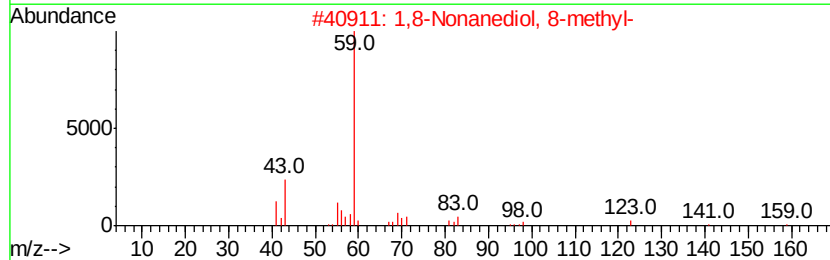
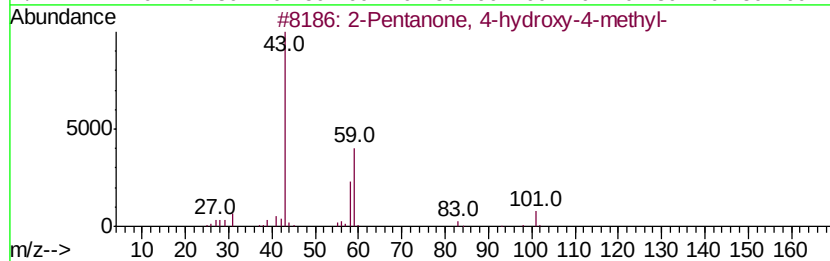
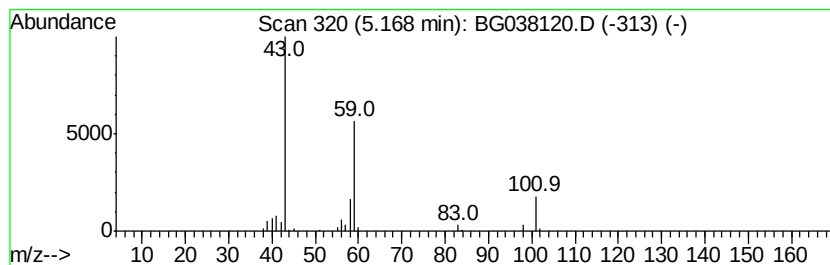
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG111318.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	4.94 ng	57511	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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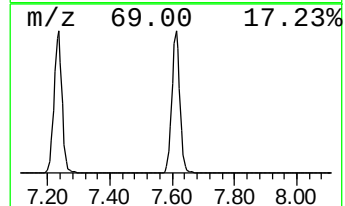
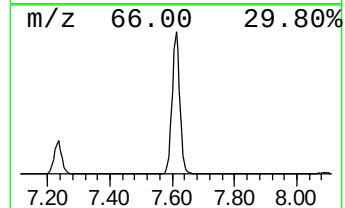
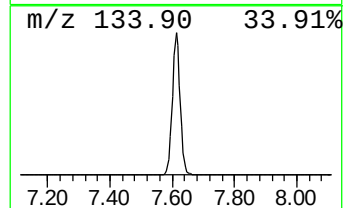
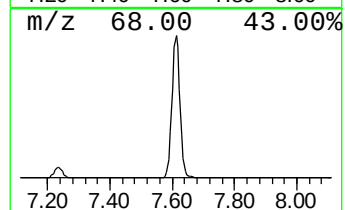
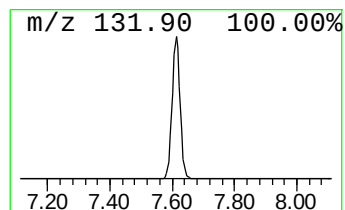
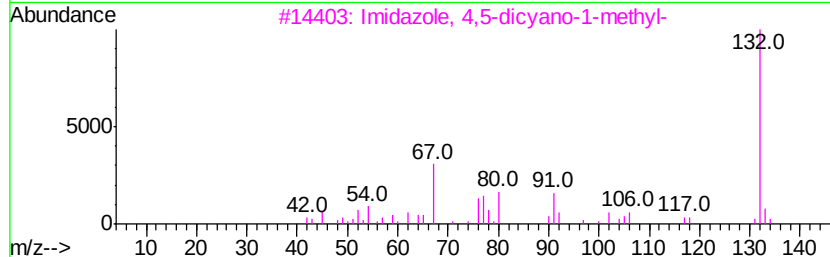
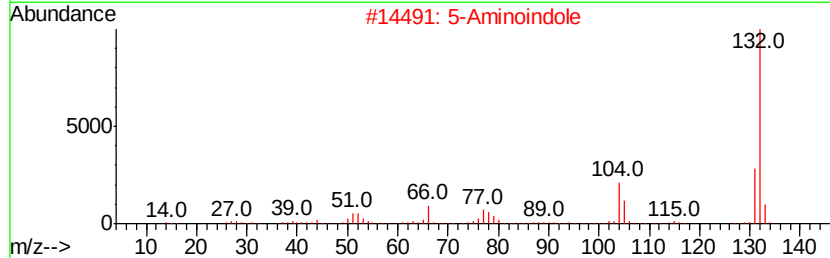
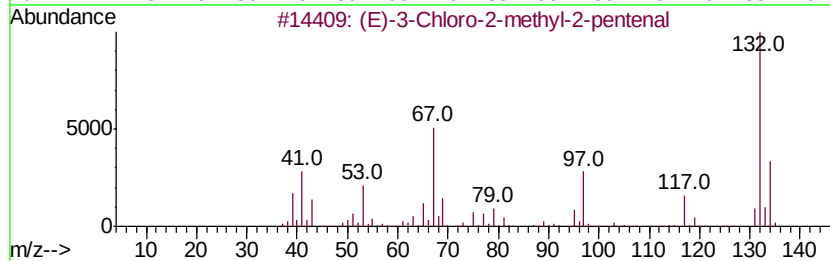
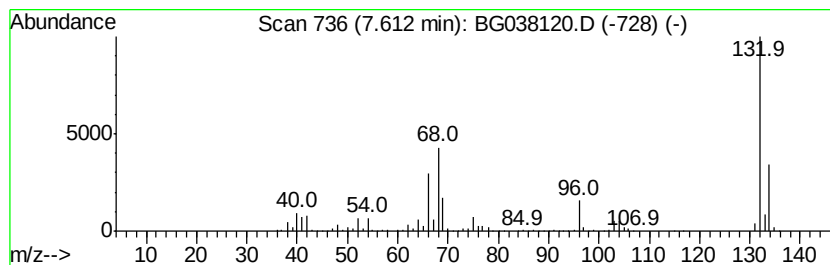
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Peak Number 2 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	101.53 ng	1182420	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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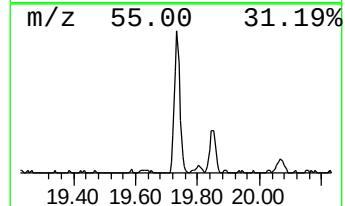
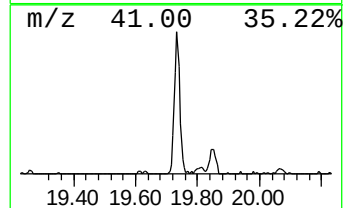
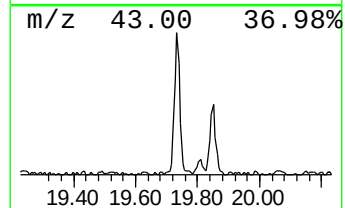
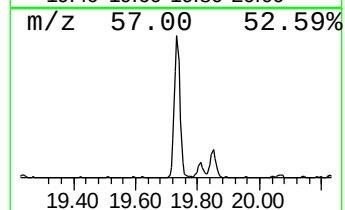
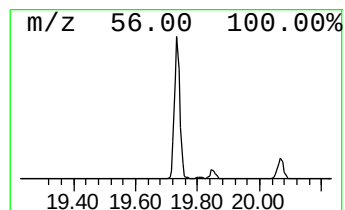
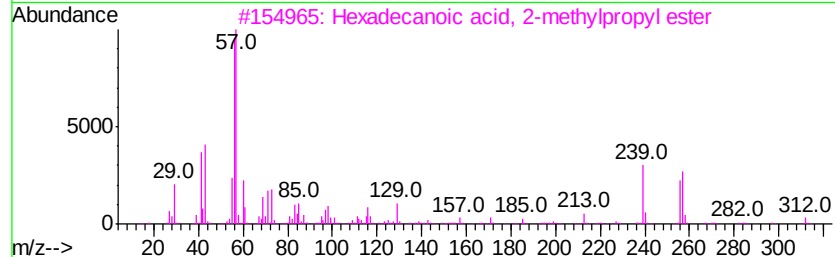
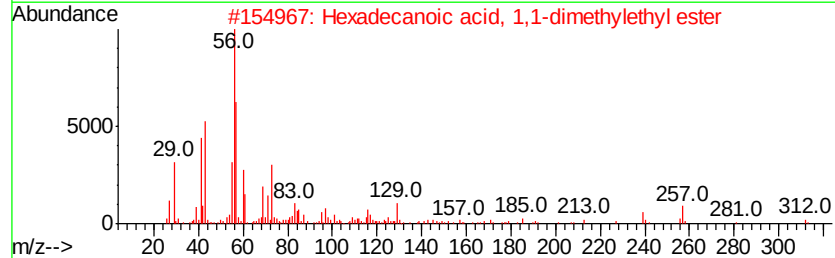
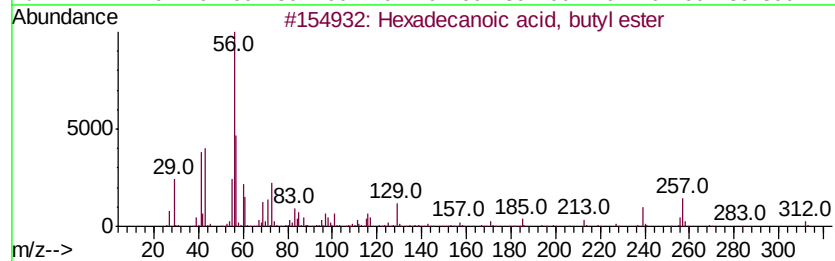
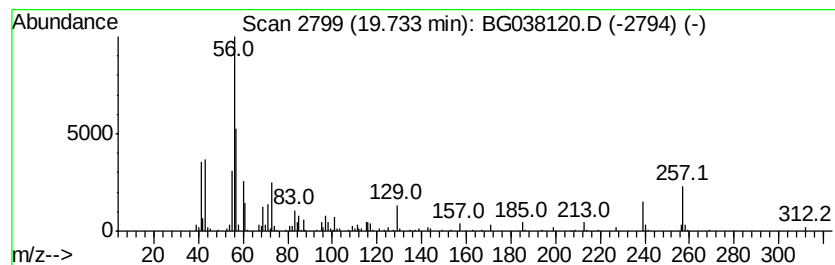
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	6.81 ng	233576	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	97
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	93
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	50
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	38



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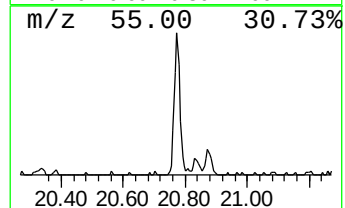
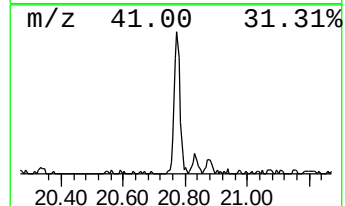
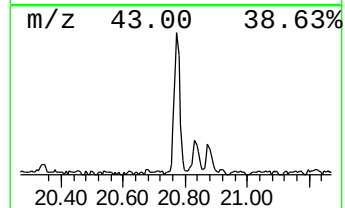
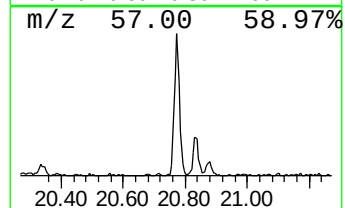
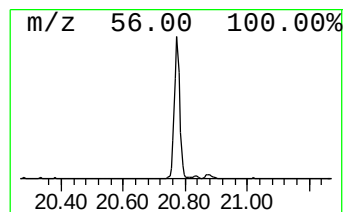
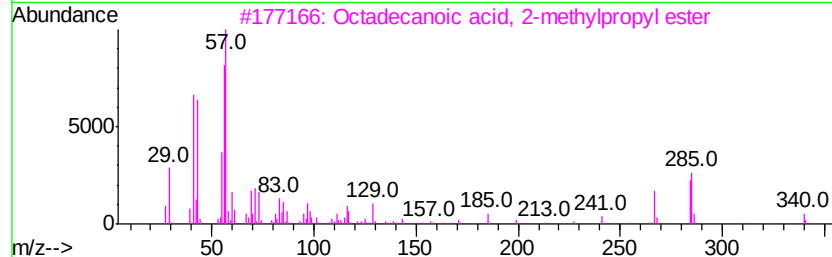
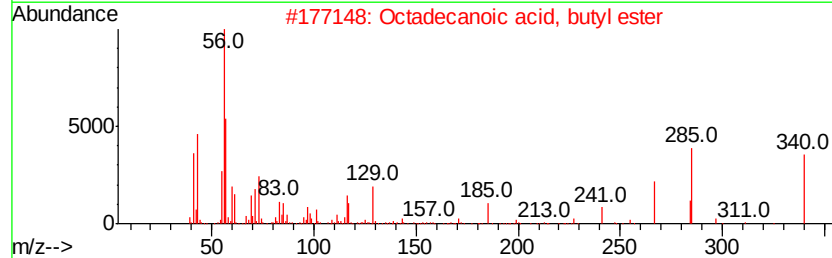
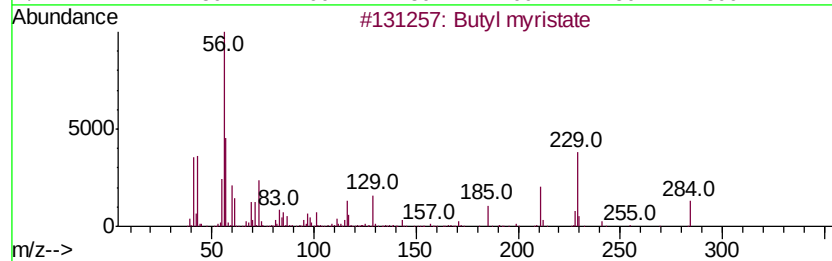
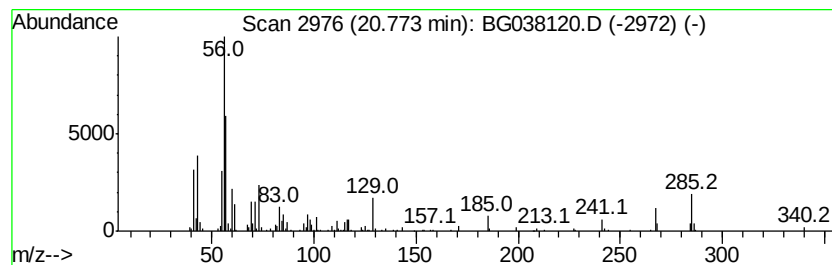
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Peak Number 5 Butyl myristate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	5.16 ng	177099	Chrysene-d12	21.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl myristate	284	C18H36O2	000110-36-1	64
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	47
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	46
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5		4-Propylcyclohexylamine	141	C9H19N	102653-37-2	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	4.9	ng	57511	1	8.09	232915	20.0
unknown7.61	7.61	101.5	ng	1182420	1	8.09	232915	20.0
Hexadecanoic acid...	19.73	6.8	ng	233576	5	21.75	686381	20.0
Butyl myristate	20.77	5.2	ng	177099	5	21.75	686381	20.0