

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081518\
 Data File : BF108187.D
 Acq On : 16 Aug 2018 1:13
 Operator : JU/SJ
 Sample : J4440-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 080918-TIPC-F-D-S

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_F\METHODS\8270-BF080818.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	2.366	3	5	14	rVB	1343010	1420691	20.26%	3.475%
2	5.248	492	495	501	rVB	72380	71961	1.03%	0.176%
3	5.637	557	561	564	rBV	2103655	1775929	25.33%	4.344%
4	6.625	725	729	732	rBV	1459091	1165056	16.62%	2.850%
5	6.784	751	756	759	rBV	3824173	3405405	48.57%	8.330%
6	7.013	791	795	799	rBV	1405622	1221409	17.42%	2.988%
7	7.172	817	822	826	rBV	4833285	4709357	67.17%	11.519%
8	7.578	885	891	894	rBV	3619531	4145196	59.12%	10.139%
9	8.301	1009	1014	1017	rBV	1606902	1531253	21.84%	3.746%
10	9.378	1190	1197	1200	rBV	6866415	7011012	100.00%	17.149%
11	9.760	1258	1262	1267	rBV	536953	448699	6.40%	1.098%
12	10.060	1309	1313	1320	rVB	1917776	1684560	24.03%	4.121%
13	10.719	1422	1425	1428	rBV	274550	202850	2.89%	0.496%
14	10.854	1443	1448	1460	rBV	2467059	2358363	33.64%	5.769%
15	10.942	1460	1463	1470	rVB2	72029	93308	1.33%	0.228%
16	11.554	1563	1567	1571	rBV	1704630	1504557	21.46%	3.680%
17	12.942	1800	1803	1806	rVB	498601	371875	5.30%	0.910%
18	13.142	1833	1837	1841	rBV	4562638	4544802	64.82%	11.117%
19	13.648	1920	1923	1927	rBV	305977	253964	3.62%	0.621%
20	14.207	2014	2018	2022	rBV	1220468	1173292	16.73%	2.870%
21	14.648	2090	2093	2098	rBV2	77220	78573	1.12%	0.192%
22	14.977	2145	2149	2154	rVB	96704	96670	1.38%	0.236%
23	15.342	2207	2211	2217	rVB	102049	115851	1.65%	0.283%
24	15.771	2277	2284	2291	rBV	855543	1261257	17.99%	3.085%
25	16.236	2359	2363	2369	rVB	79012	120886	1.72%	0.296%
26	16.795	2453	2458	2469	rVB	61482	115310	1.64%	0.282%

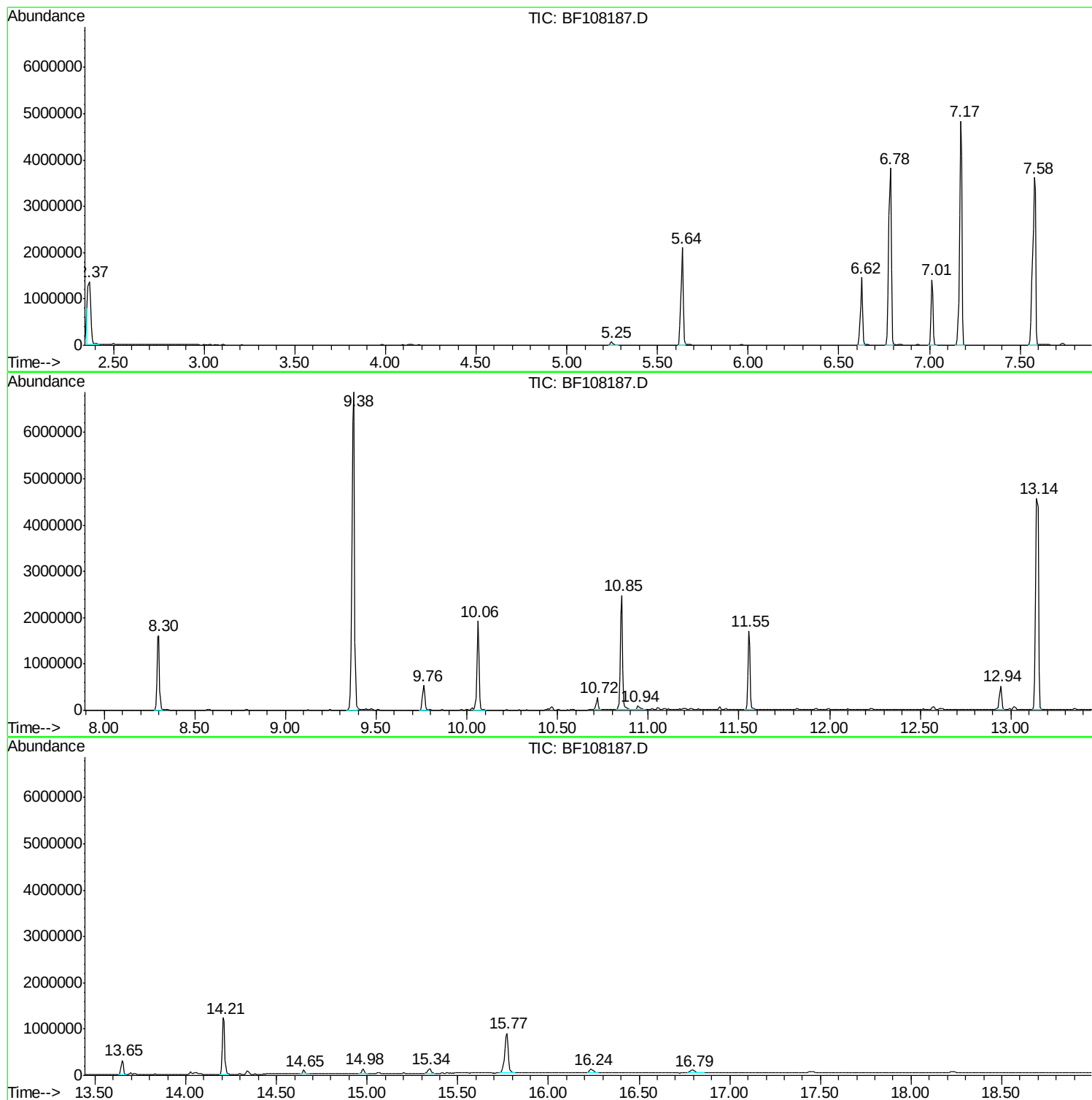
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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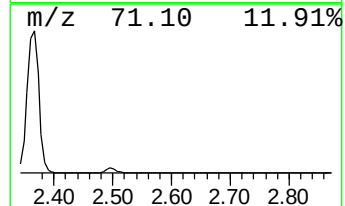
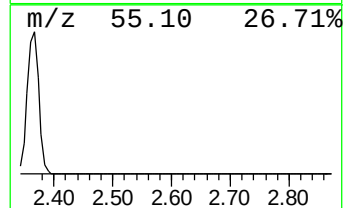
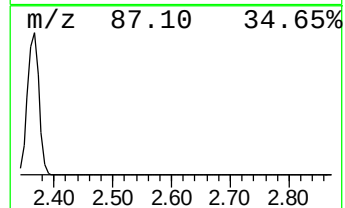
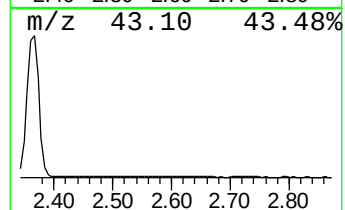
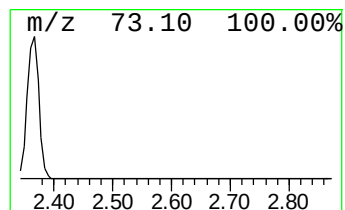
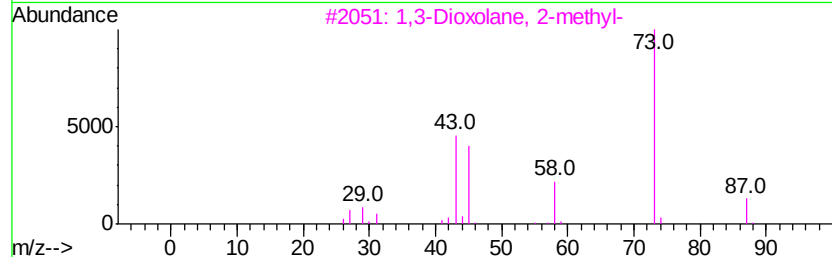
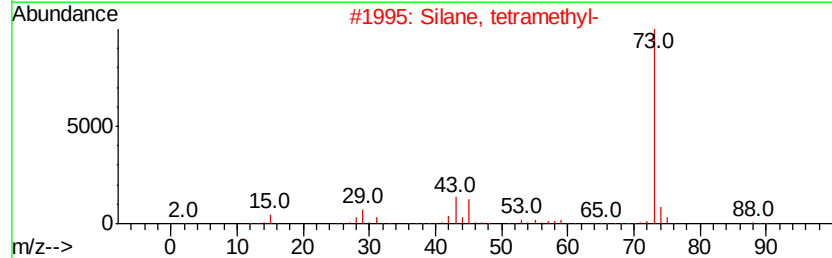
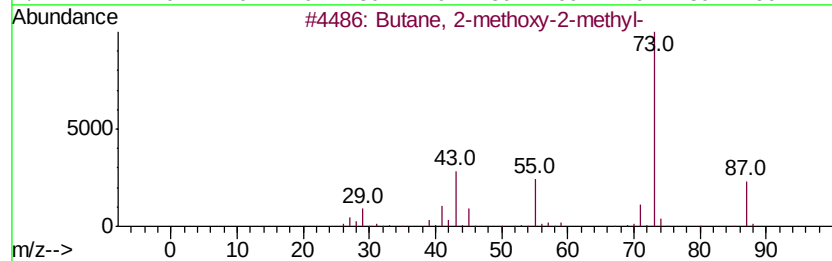
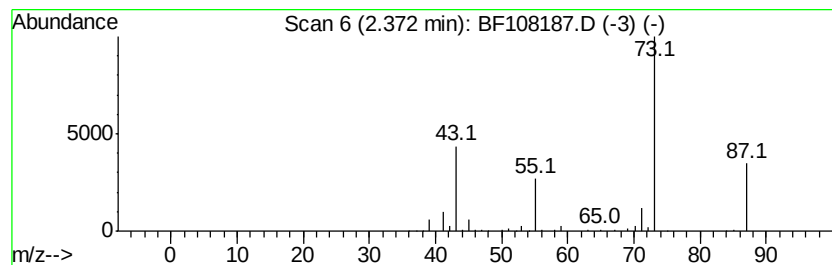
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	23.26 ng	1420690	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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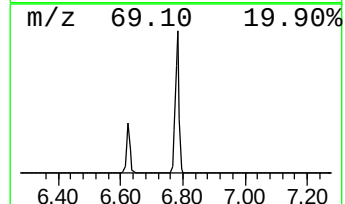
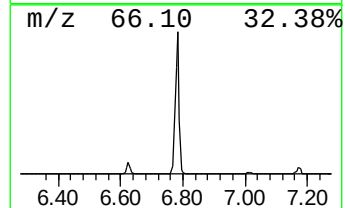
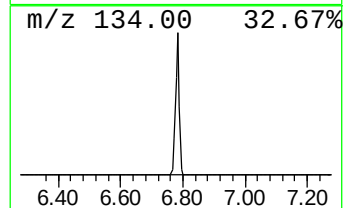
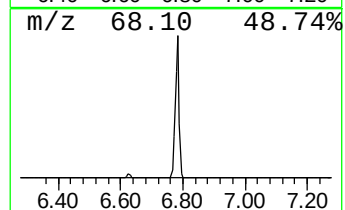
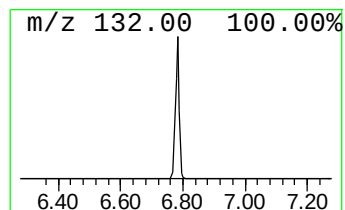
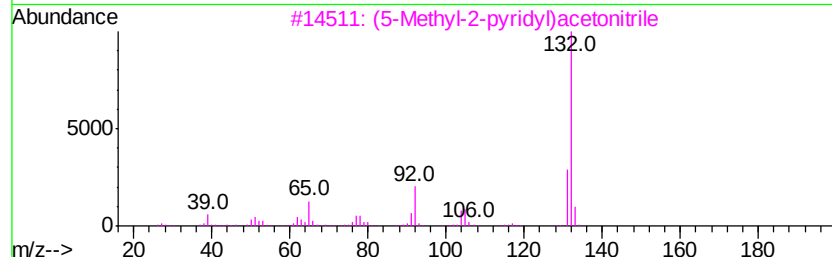
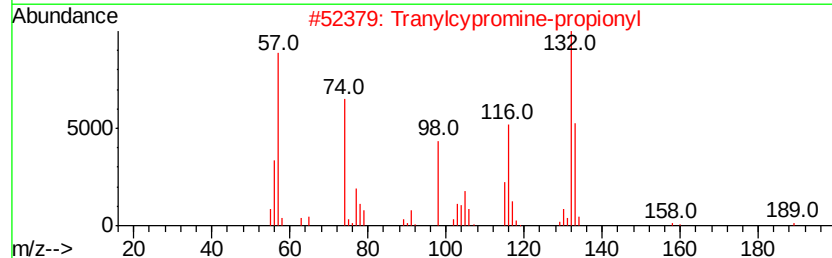
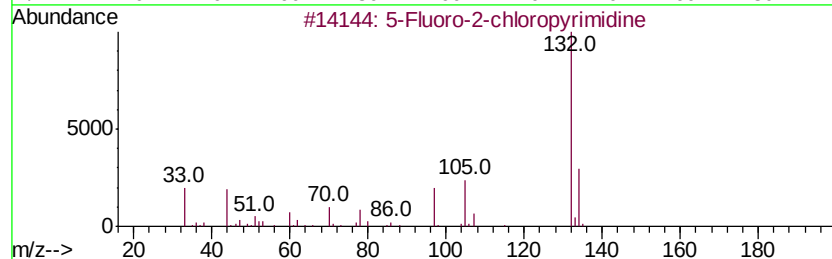
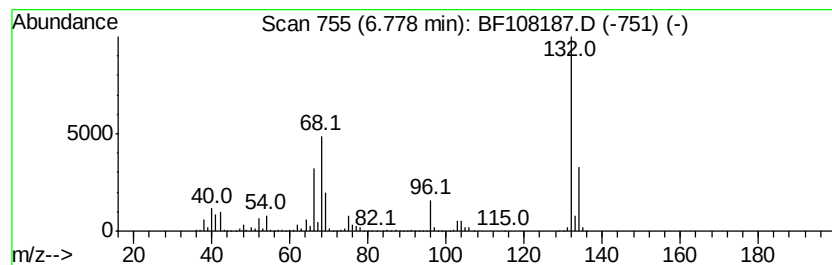
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Peak Number 2 unknown6.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	55.76 ng	3405410	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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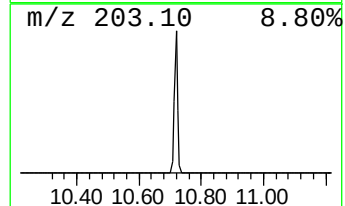
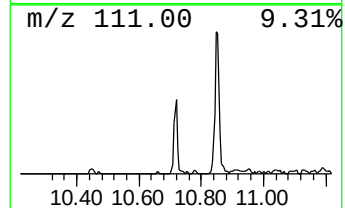
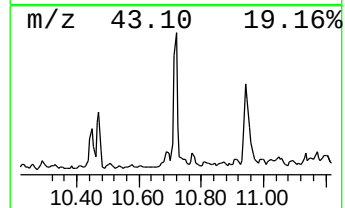
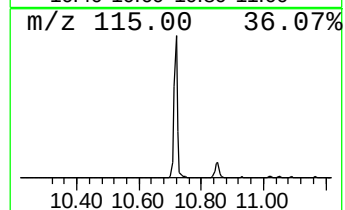
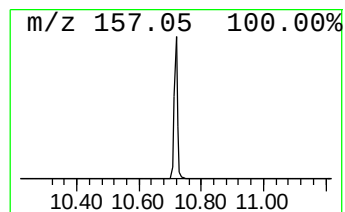
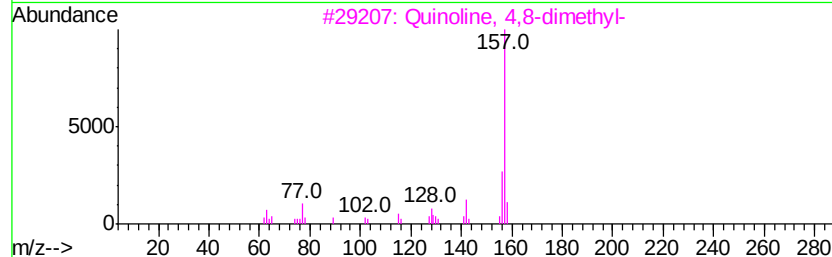
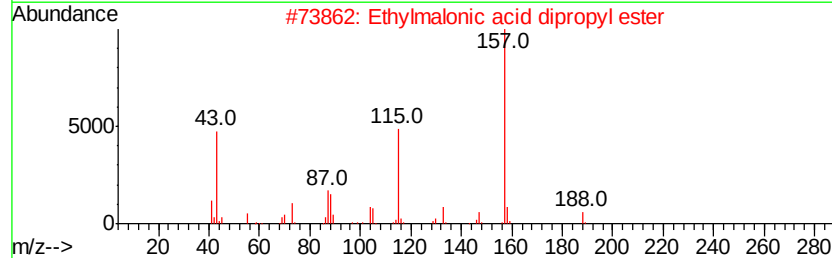
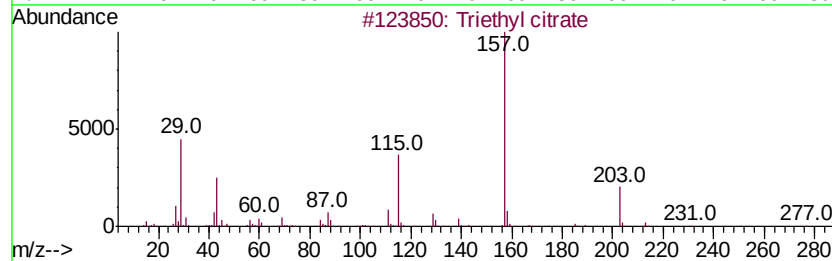
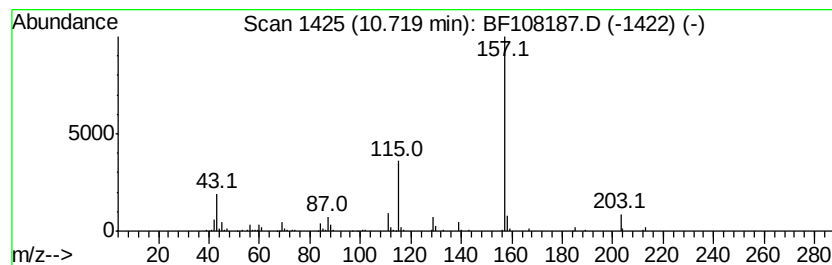
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BNA_F
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Peak Number 4 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.72	2.41 ng	202850	Acenaphthene-d10		10.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	45
3	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
4	4-Fluoro-2-nitrophenol	157	C6H4FN03	000394-33-2	36
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36



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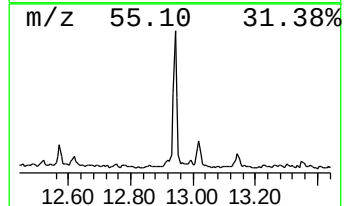
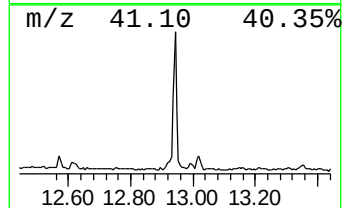
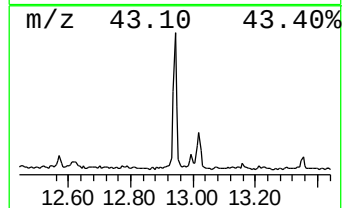
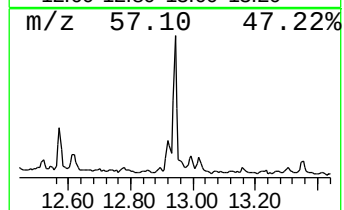
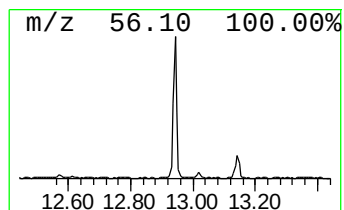
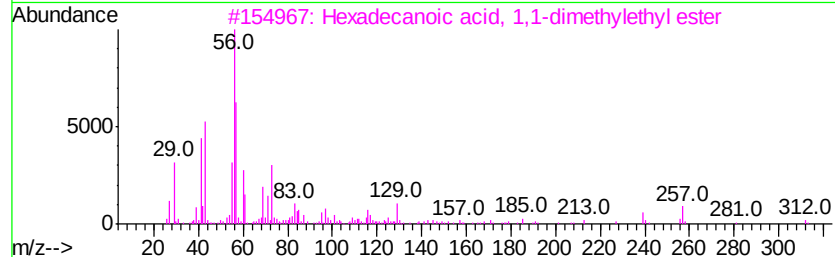
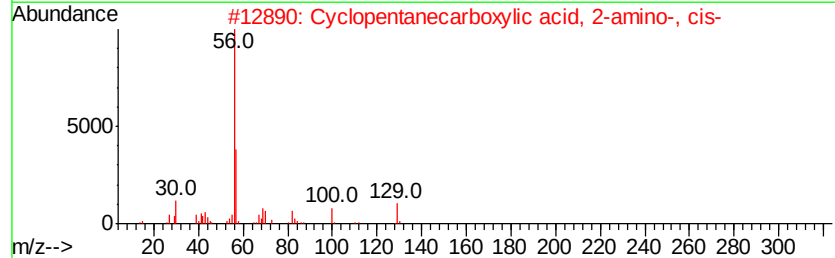
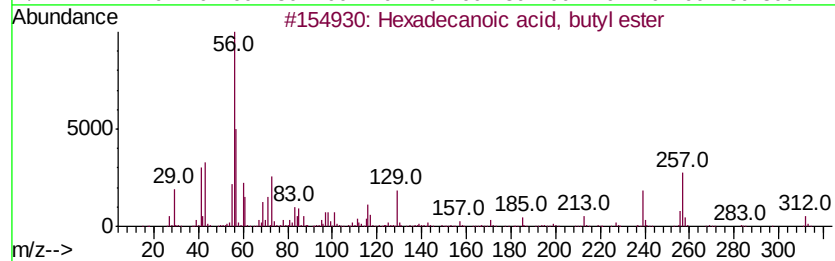
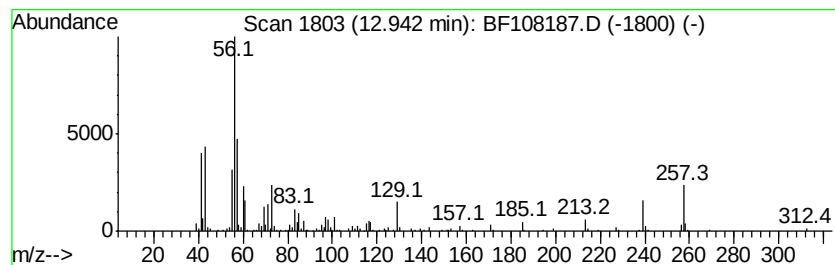
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	6.34 ng	371875	Chrysene-d12	14.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
4		Cyclopentanamine	85	C5H11N	001003-03-8	35
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	32



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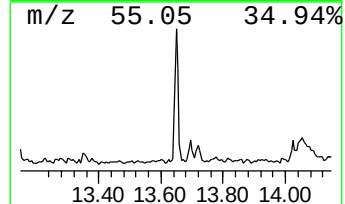
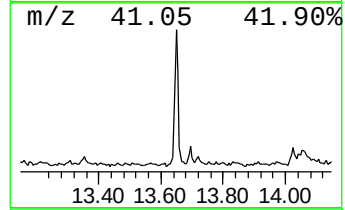
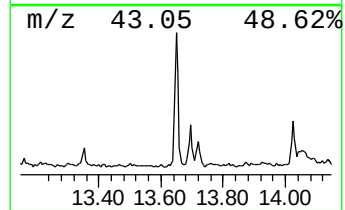
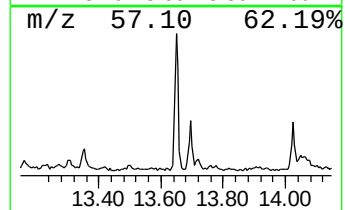
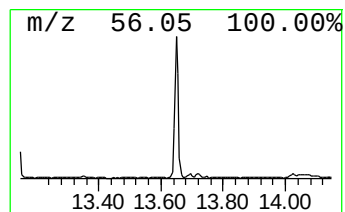
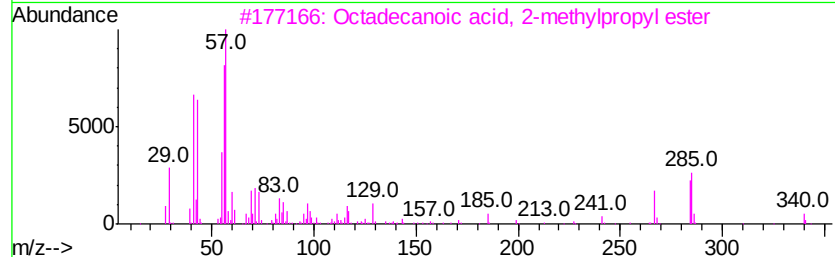
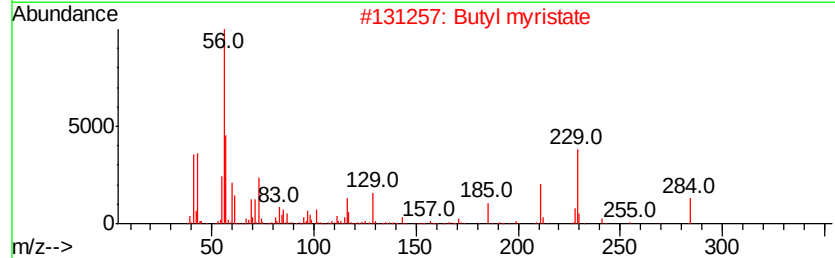
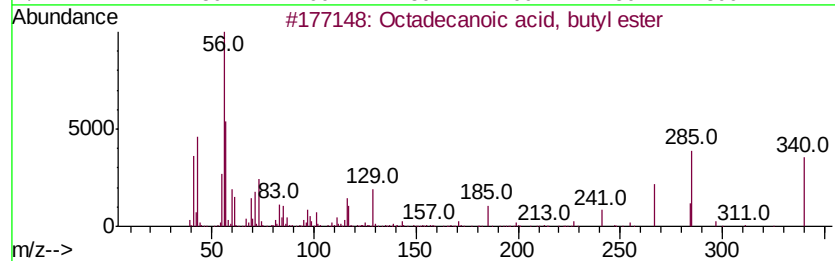
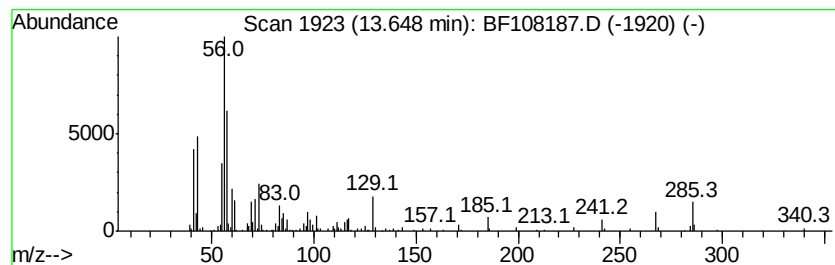
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	4.33 ng	253964	Chrysene-d12	14.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	72
3		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	38
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.37	23.3	ng	1420690	1	7.01	1221410	20.0
unknown6.78	6.78	55.8	ng	3405410	1	7.01	1221410	20.0
Triethyl citrate	10.72	2.4	ng	202850	3	10.06	1684560	20.0
Hexadecanoic acid...	12.94	6.3	ng	371875	5	14.21	1173290	20.0
Octadecanoic acid...	13.65	4.3	ng	253964	5	14.21	1173290	20.0