

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108451.D
 Acq On : 24 Aug 2018 5:58
 Operator : JU/SJ
 Sample : J4582-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082018-DBRI-E-D-M

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_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	2.372	3	6	22	rVB	2356275	2957551	69.85%	11.256%
2	5.237	489	493	499	rBV	67312	75155	1.78%	0.286%
3	5.625	555	559	569	rBV	1215395	1127796	26.64%	4.292%
4	6.613	723	727	742	rBV	877400	793421	18.74%	3.020%
5	6.766	749	753	757	rBV	2284095	2071496	48.92%	7.884%
6	7.001	789	793	796	rBV	846743	798502	18.86%	3.039%
7	7.160	815	820	823	rBV	2825795	2808250	66.32%	10.688%
8	7.566	883	889	892	rBV	2343103	2382419	56.27%	9.068%
9	8.283	1006	1011	1014	rBV	1105584	951628	22.48%	3.622%
10	9.360	1188	1194	1197	rBV	4536033	4234081	100.00%	16.115%
11	9.748	1256	1260	1269	rBV	128581	130392	3.08%	0.496%
12	10.042	1307	1310	1318	rVB	1118530	1027116	24.26%	3.909%
13	10.701	1419	1422	1425	rBV	184430	137043	3.24%	0.522%
14	10.836	1441	1445	1456	rBV	1471260	1341153	31.68%	5.104%
15	10.942	1458	1463	1472	rVB2	31782	58305	1.38%	0.222%
16	11.536	1561	1564	1573	rVB	896801	867541	20.49%	3.302%
17	13.124	1829	1834	1837	rBV	3186540	2790865	65.91%	10.622%
18	14.112	1995	2002	2003	rBV5	25213	46375	1.10%	0.177%
19	14.189	2011	2015	2022	rVB	854094	752675	17.78%	2.865%
20	15.742	2272	2279	2288	rBV	461795	700915	16.55%	2.668%
21	16.195	2352	2356	2364	rVB2	50907	84906	2.01%	0.323%
22	16.748	2444	2450	2455	rBV3	40221	81208	1.92%	0.309%
23	17.401	2556	2561	2567	rVB5	26067	55418	1.31%	0.211%

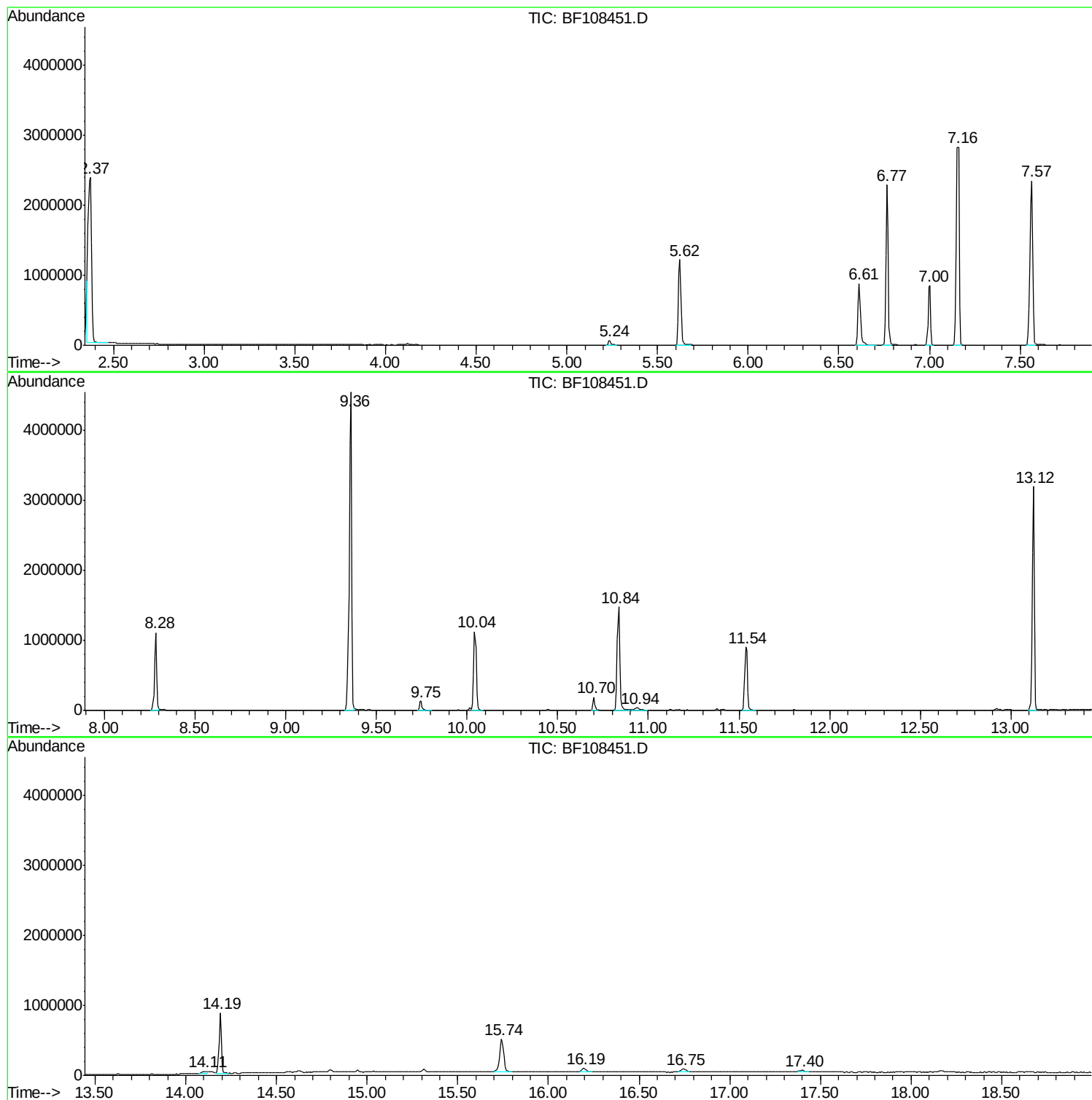
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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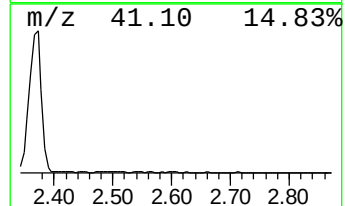
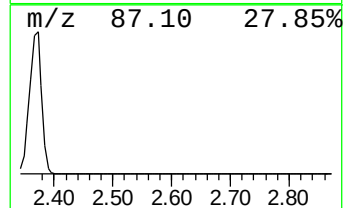
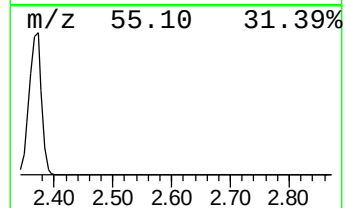
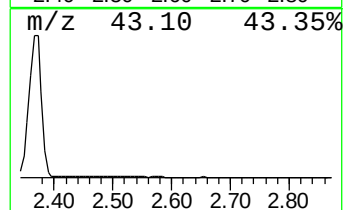
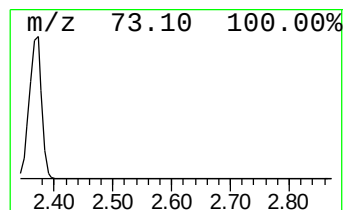
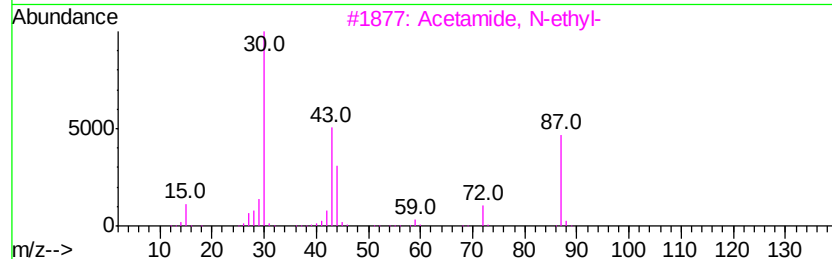
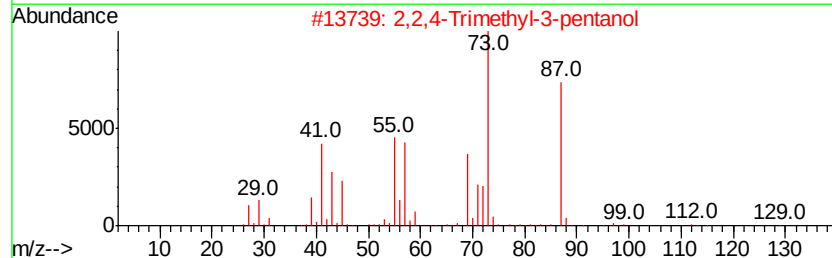
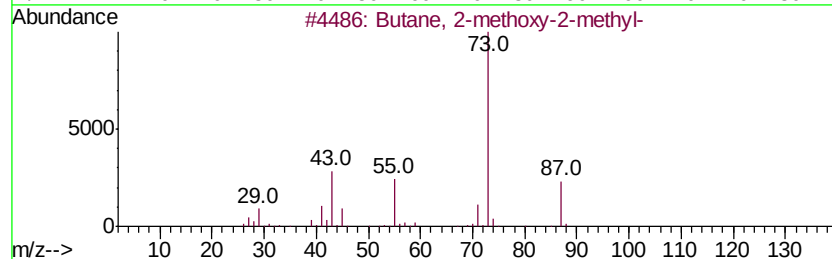
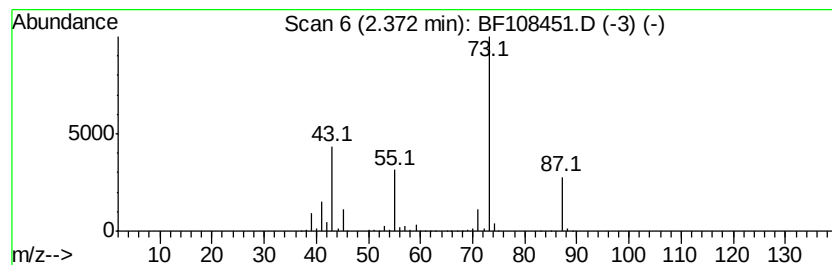
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	74.08 ng	2957550	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12



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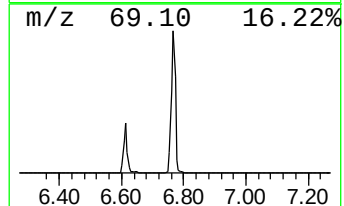
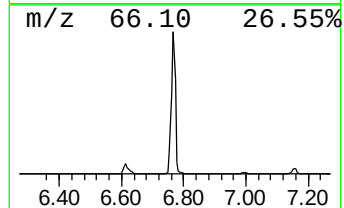
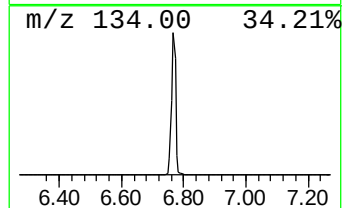
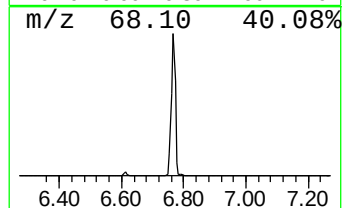
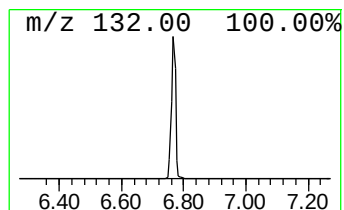
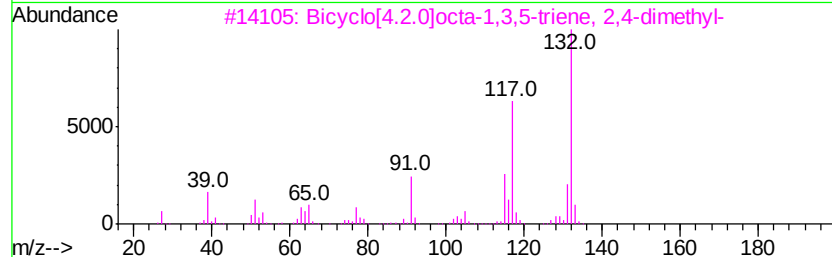
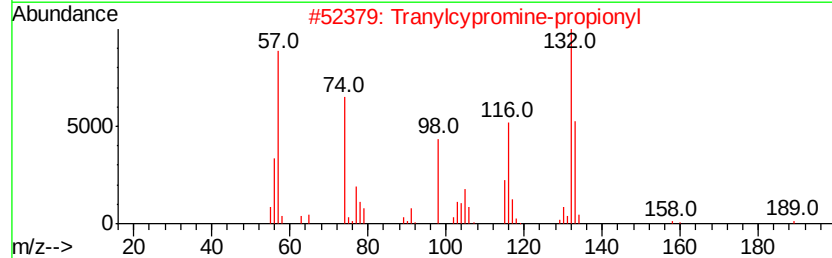
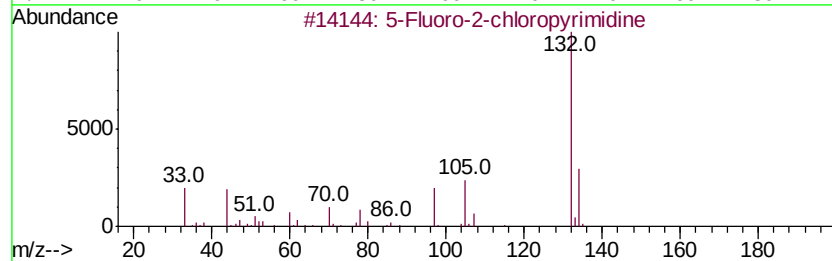
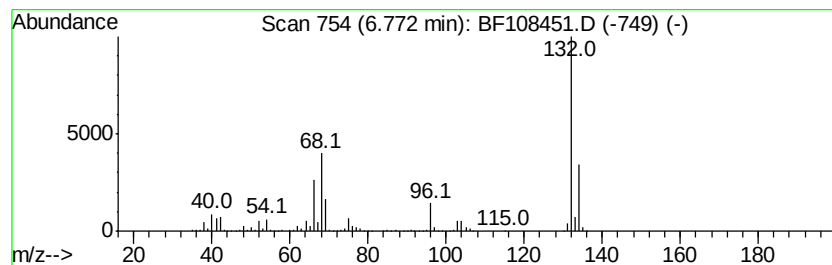
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Peak Number 2 unknown6.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	51.88 ng	2071500	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5			Xenon	132	Xe	007440-63-3	9



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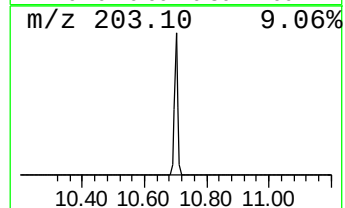
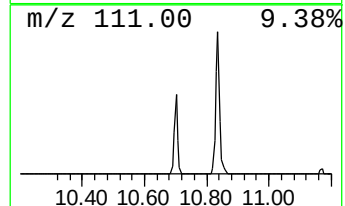
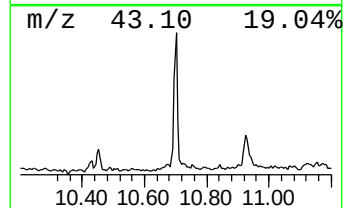
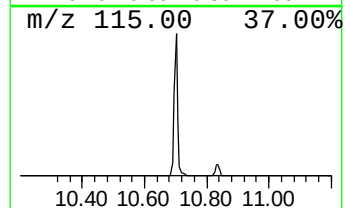
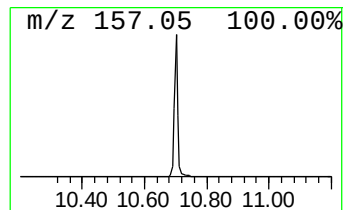
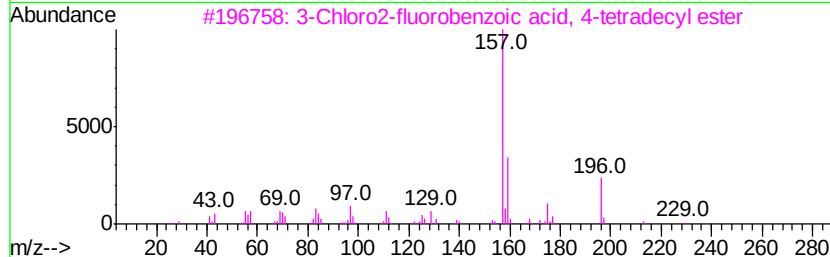
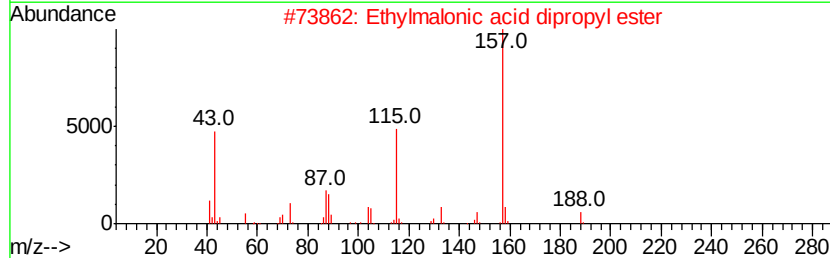
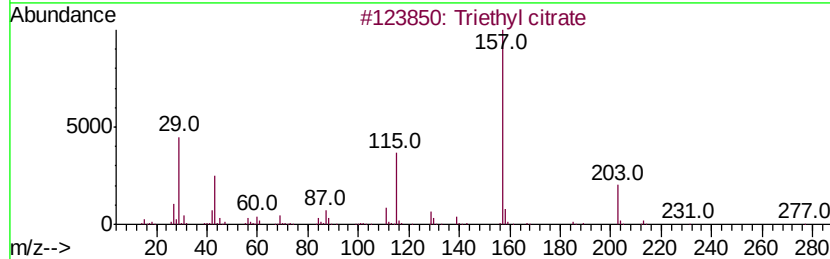
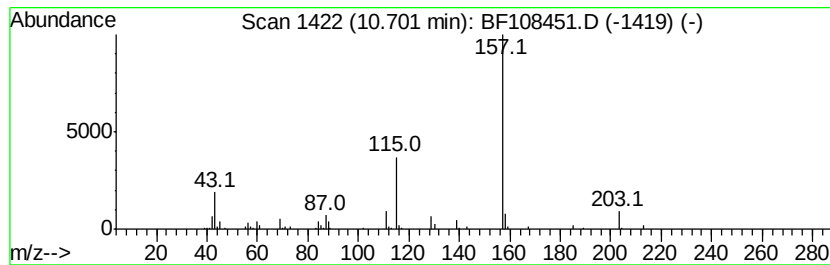
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Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.70	2.67 ng	137043	Acenaphthene-d10	10.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClF02	1000338-64-7	42
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	40
5	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	38



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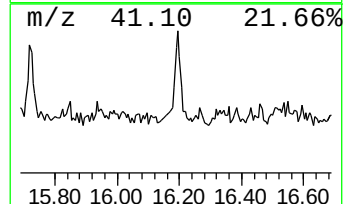
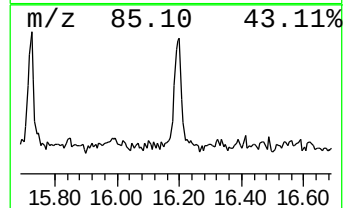
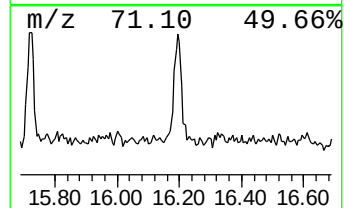
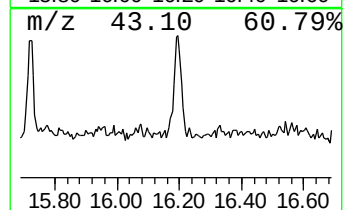
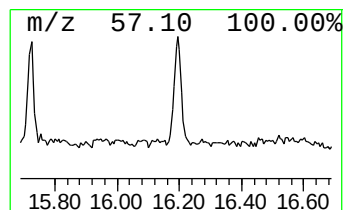
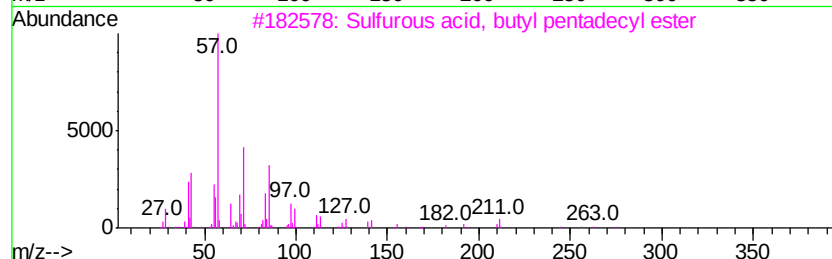
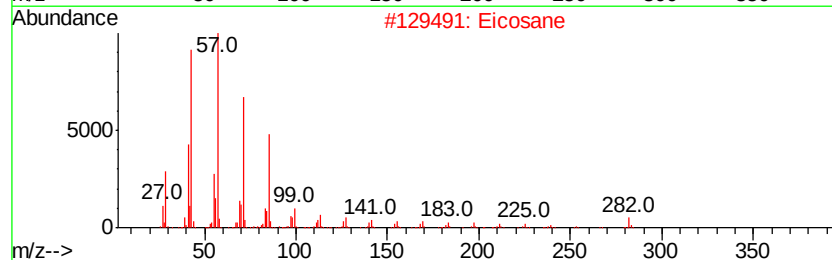
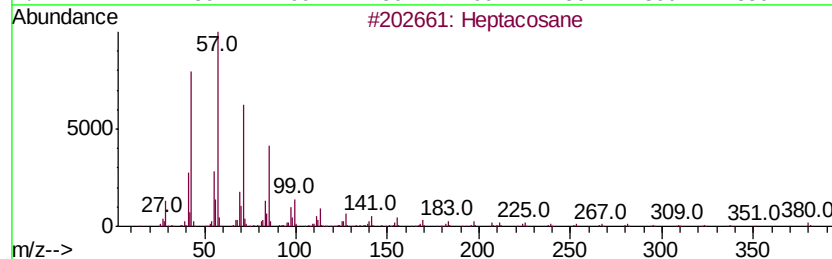
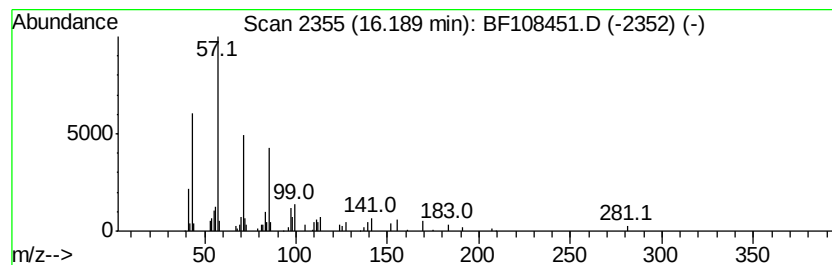
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.42 ng	84906	Perylene-d12	15.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	87
2	Eicosane		282	C20H42	000112-95-8	87
3	Sulfurous acid, butyl pentadecyl...		348	C19H40O3S	1000309-18-2	86
4	Triacontane		422	C30H62	000638-68-6	86
5	Hentriacontane		437	C31H64	000630-04-6	86



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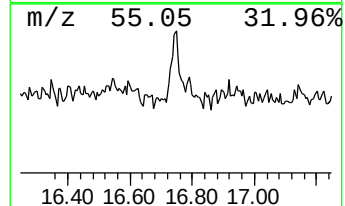
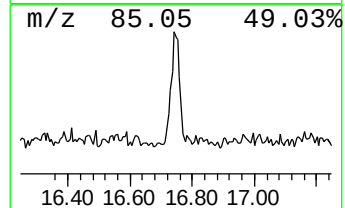
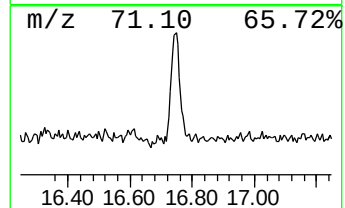
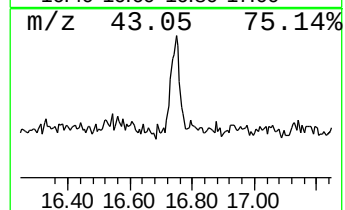
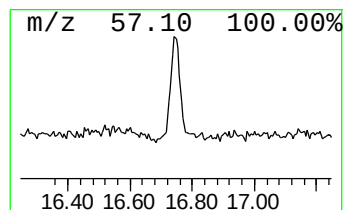
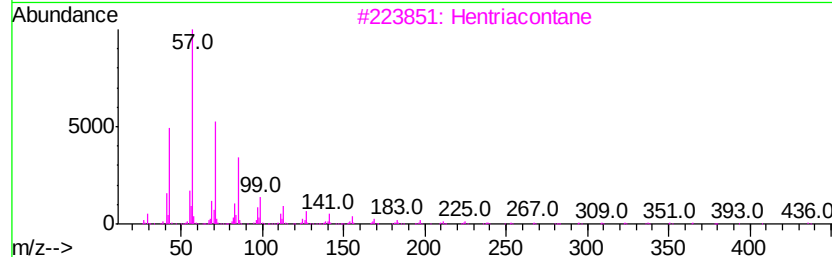
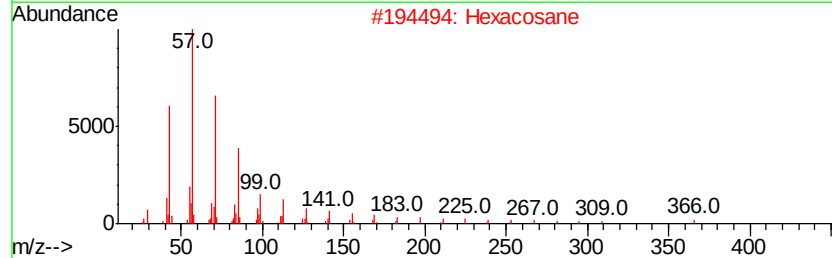
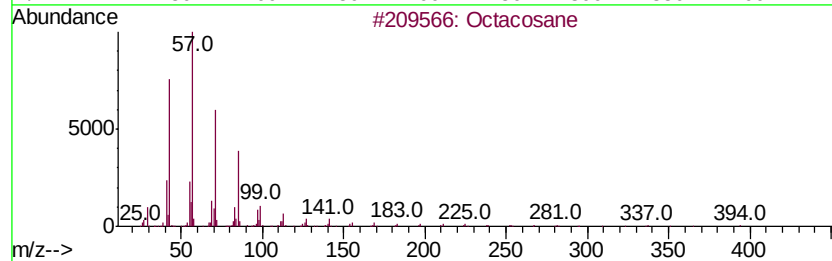
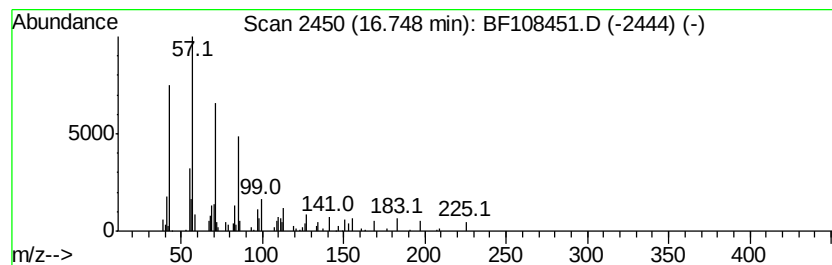
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Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.32 ng	81208	Perylene-d12	15.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Hexacosane		366	C26H54	000630-01-3	90
3	Hentriacontane		437	C31H64	000630-04-6	90
4	Tetratetracontane		619	C44H90	007098-22-8	90
5	Eicosane, 10-methyl-		296	C21H44	054833-23-7	87



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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
Butane, 2-methoxy...	2.37	74.1	ng	2957550	1	7.00	798502	20.0
unknown6.77	6.77	51.9	ng	2071500	1	7.00	798502	20.0
Triethyl citrate	10.70	2.7	ng	137043	3	10.04	1027120	20.0
Heptacosane	16.19	2.4	ng	84906	6	15.74	700915	20.0
Octacosane	16.75	2.3	ng	81208	6	15.74	700915	20.0