

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082416\
 Data File : BF089875.D
 Acq On : 24 Aug 2016 15:35
 Operator : UM/SJ
 Sample : H4551-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AST-6

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:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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	1.655	4	6	14	rVV	1331106	2284926	9.40%	1.688%
2	1.770	14	16	72	rVB	9300333	24297198	100.00%	17.948%
3	4.799	278	281	291	rBV	1608585	2453347	10.10%	1.812%
4	5.244	317	320	322	rBV	8061831	8861297	36.47%	6.546%
5	6.307	409	413	415	rBV	7999579	9531345	39.23%	7.041%
6	6.433	421	424	426	rBV	9348886	9639280	39.67%	7.120%
7	6.662	442	444	446	rBV	2639822	2458950	10.12%	1.816%
8	6.822	455	458	460	rBV	8356135	7086490	29.17%	5.235%
9	7.233	491	494	496	rBV	6020684	5831139	24.00%	4.307%
10	7.953	554	557	559	rBV	3991745	3465055	14.26%	2.560%
11	9.039	649	652	654	rBV	10074414	11289330	46.46%	8.339%
12	9.428	684	686	689	rBV	2595842	2505997	10.31%	1.851%
13	9.702	708	710	712	rBV	4146635	3693501	15.20%	2.728%
14	10.491	776	779	781	rBV	5077206	5548762	22.84%	4.099%
15	10.628	789	791	796	rVB	312172	341762	1.41%	0.252%
16	11.176	837	839	843	rBV2	3745823	5162545	21.25%	3.813%
17	11.256	843	846	847	rVB2	233945	352552	1.45%	0.260%
18	11.405	856	859	861	rBV	271886	280230	1.15%	0.207%
19	11.702	884	885	887	rVV	218039	247519	1.02%	0.183%
20	11.759	887	890	891	rVV	386407	461662	1.90%	0.341%
21	11.782	891	892	897	rVB	213921	402819	1.66%	0.298%
22	11.976	907	909	913	rVB2	163552	250434	1.03%	0.185%
23	12.388	942	945	947	rBV	2598738	2565456	10.56%	1.895%
24	12.616	961	965	967	rVV	1810575	2449398	10.08%	1.809%
25	12.777	977	979	982	rVV	8097335	8521501	35.07%	6.295%
26	12.948	989	994	996	rVB	321406	496679	2.04%	0.367%
27	13.051	1001	1003	1008	rVV3	200224	352359	1.45%	0.260%
28	13.474	1037	1040	1043	rVB	195818	243118	1.00%	0.180%
29	13.588	1048	1050	1052	rBV	177305	255312	1.05%	0.189%
30	13.622	1052	1053	1058	rBV3	117466	298872	1.23%	0.221%
31	13.748	1062	1064	1070	rBV2	237606	631352	2.60%	0.466%
32	13.862	1071	1074	1079	rVV2	3346524	5428318	22.34%	4.010%
33	14.445	1122	1125	1130	rBV4	122818	292263	1.20%	0.216%
34	14.982	1169	1172	1177	rBV	815510	1608312	6.62%	1.188%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.268	1194	1197	1199	rVB	392442	492369	2.03%	0.364%
36	15.314	1199	1201	1204	rVB	479553	638705	2.63%	0.472%
37	15.382	1204	1207	1209	rBV	1962407	2669867	10.99%	1.972%
38	16.663	1316	1319	1324	rVB2	206863	442747	1.82%	0.327%
39	17.040	1346	1352	1360	rVB	200789	502007	2.07%	0.371%
40	18.994	1516	1523	1531	rVB2	336547	1043962	4.30%	0.771%

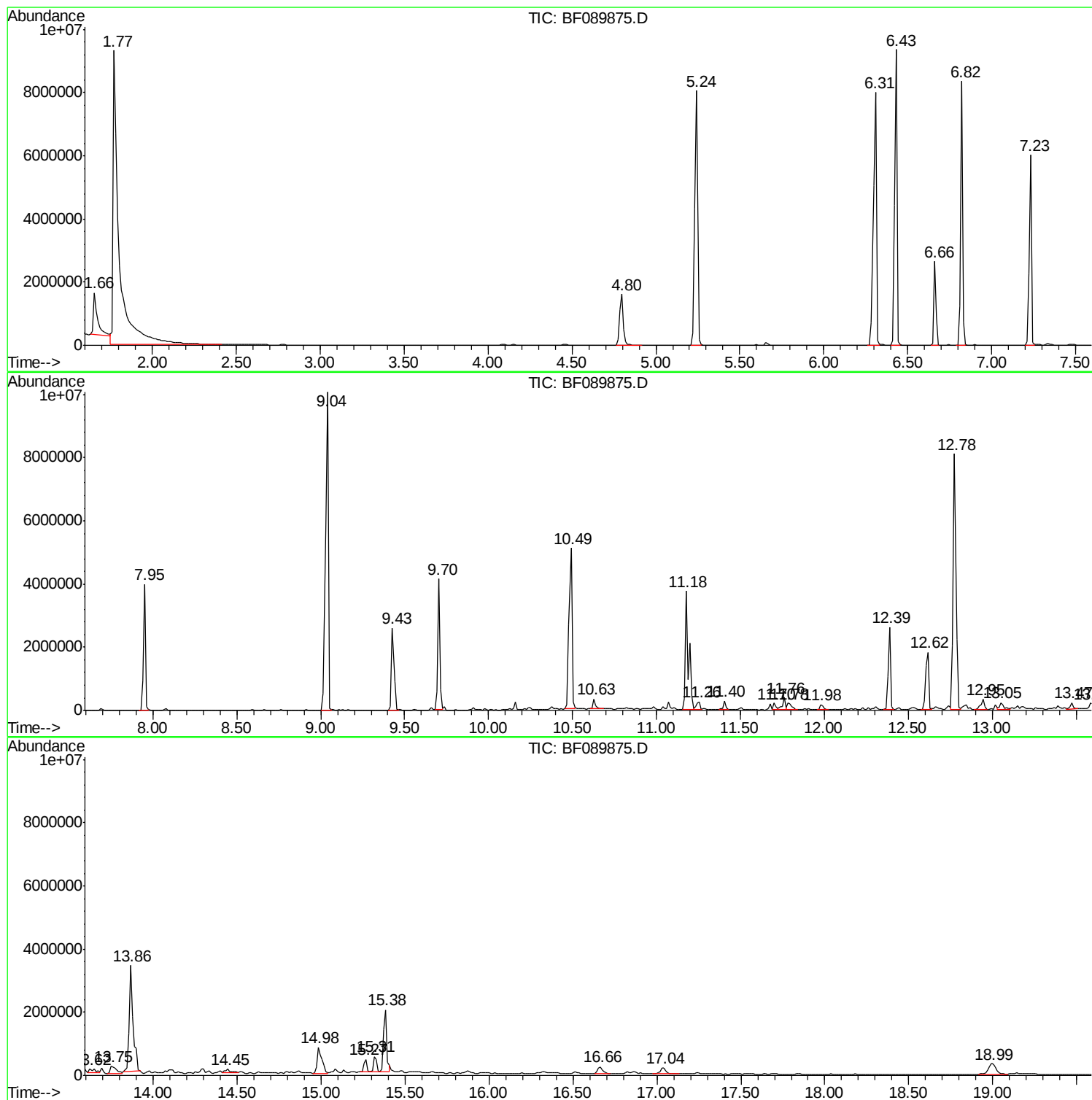
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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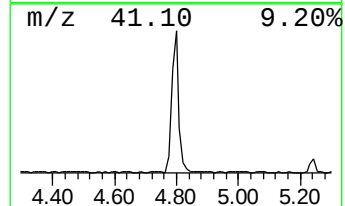
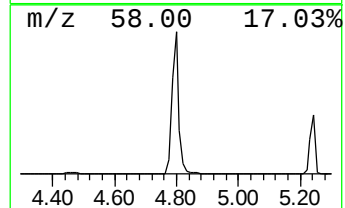
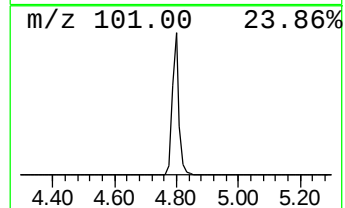
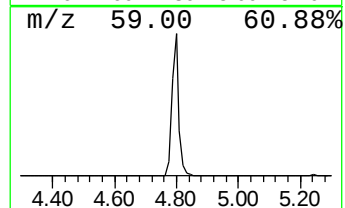
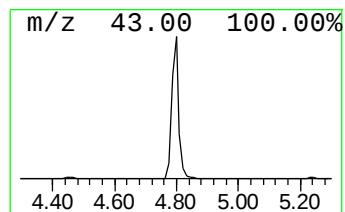
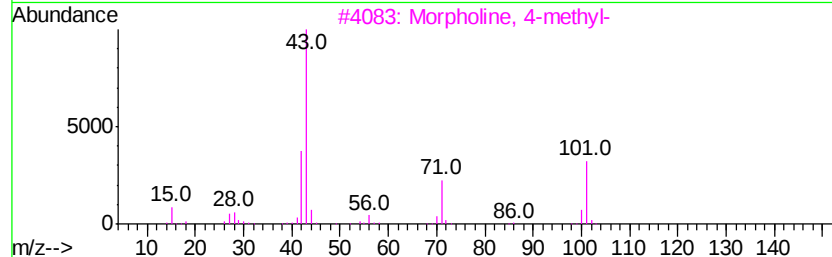
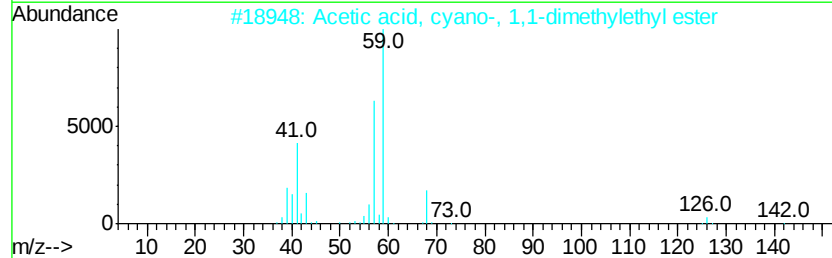
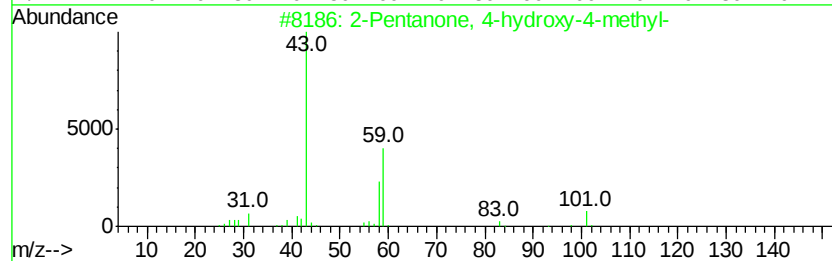
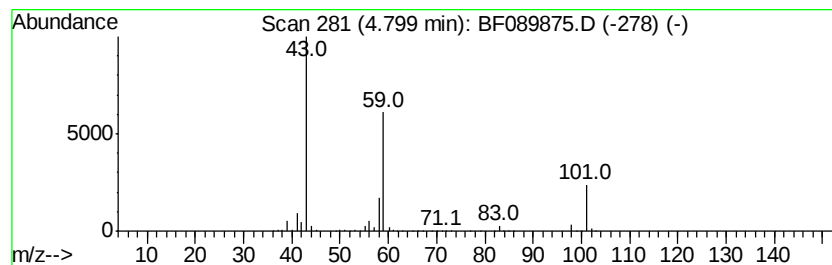
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	19.95 ng	2453350	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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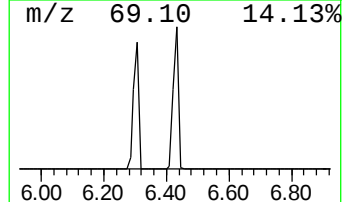
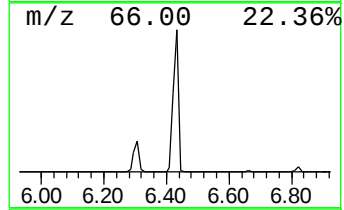
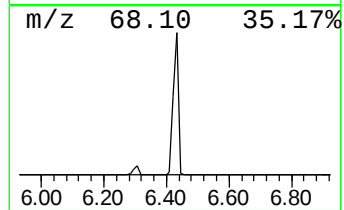
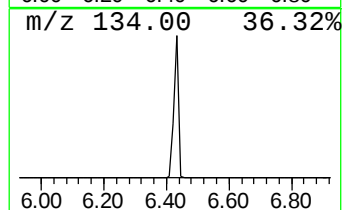
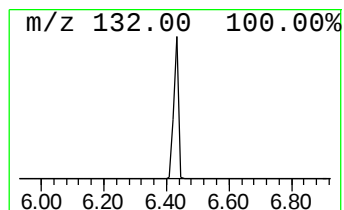
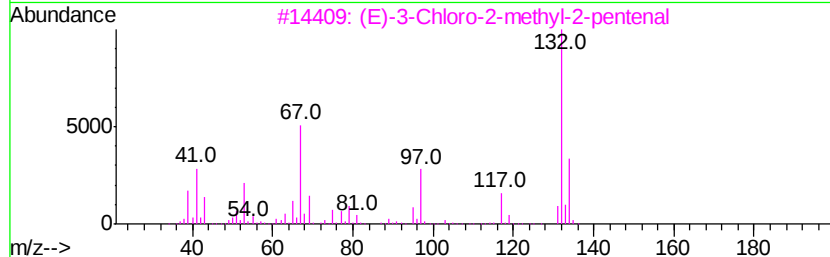
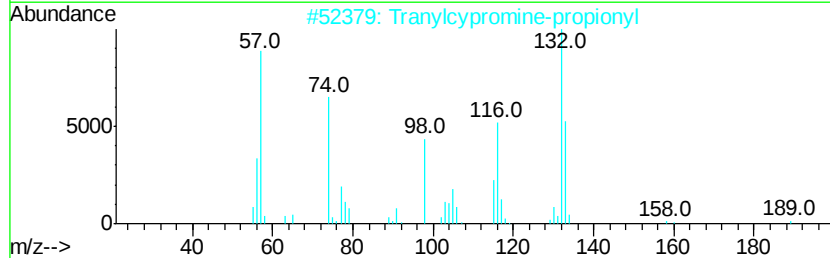
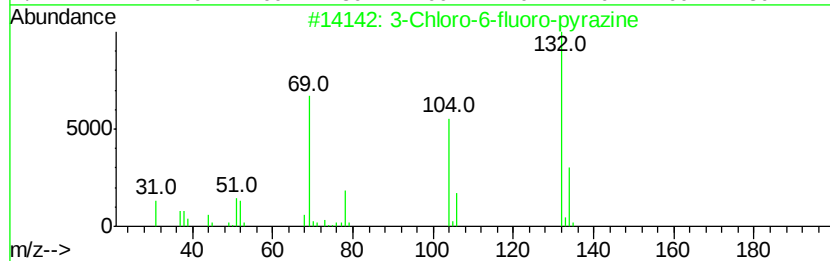
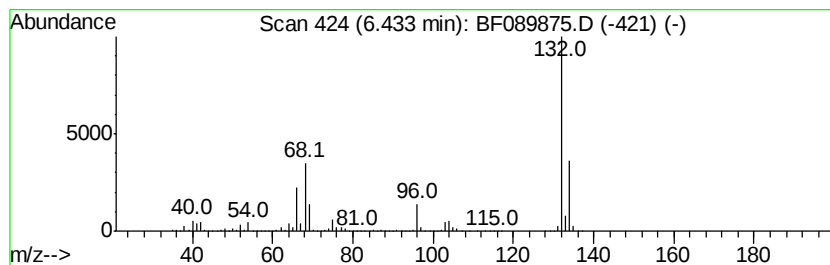
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Peak Number 4 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	78.40 ng	9639280	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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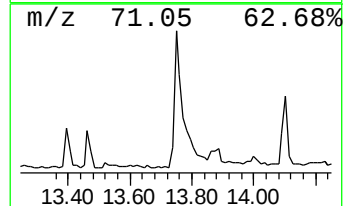
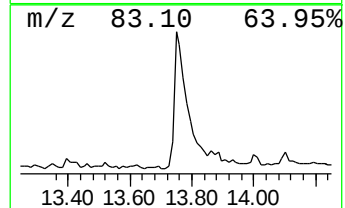
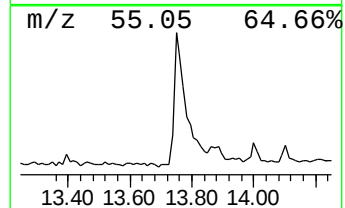
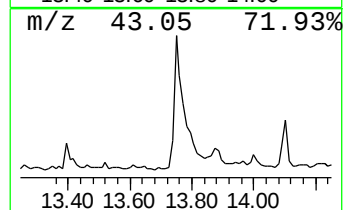
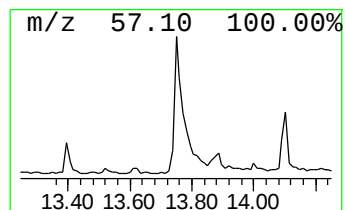
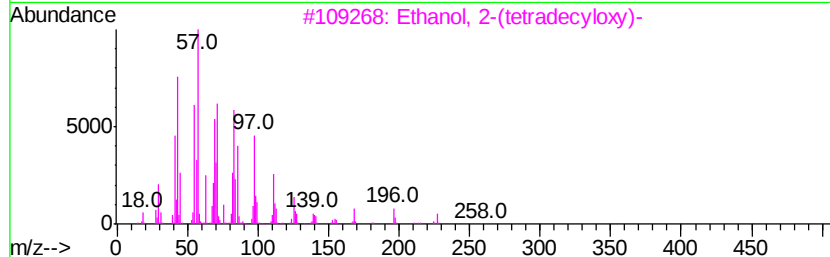
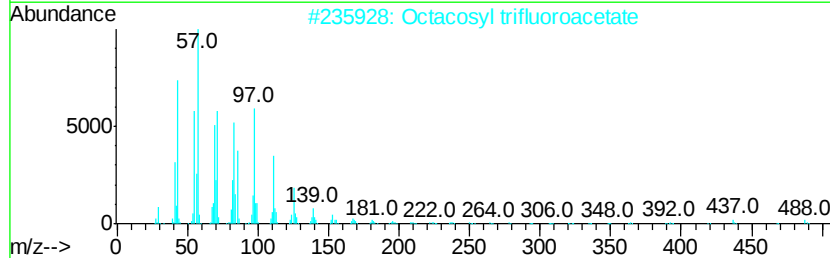
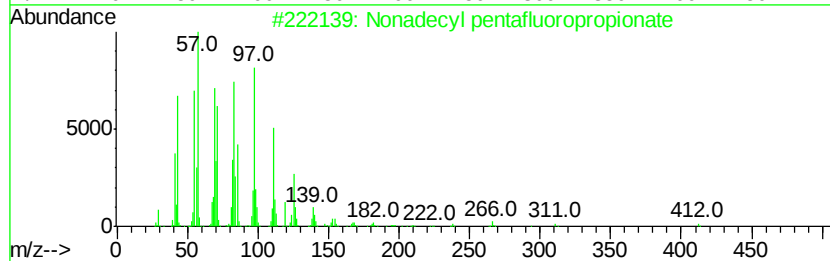
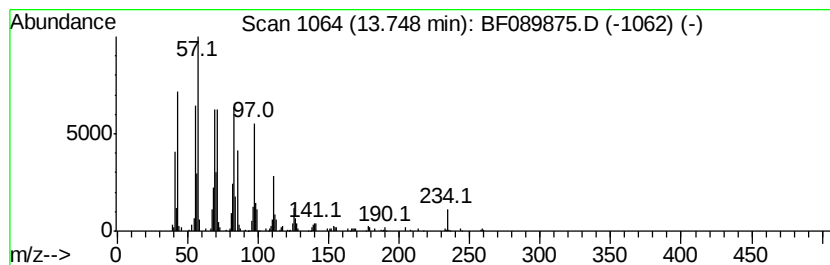
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Peak Number 6 Nonadecyl pentafluoropropio... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.33 ng	631352	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81



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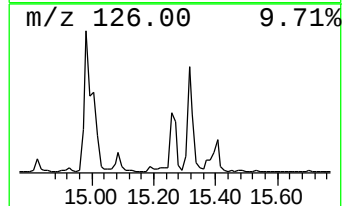
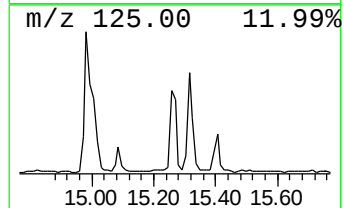
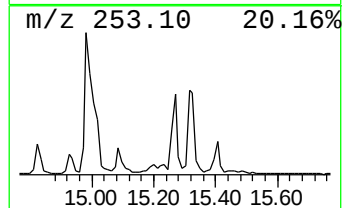
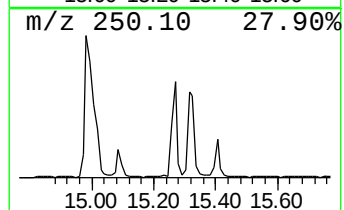
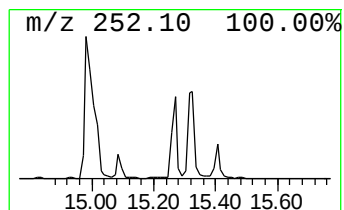
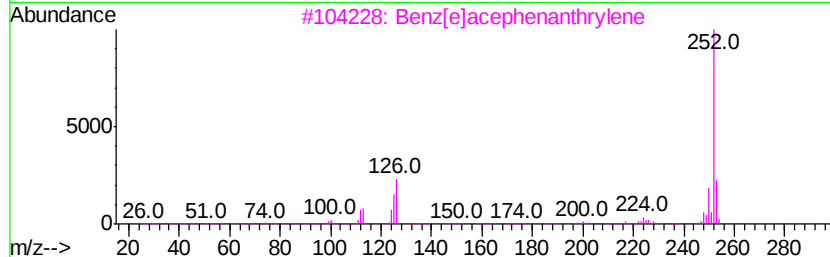
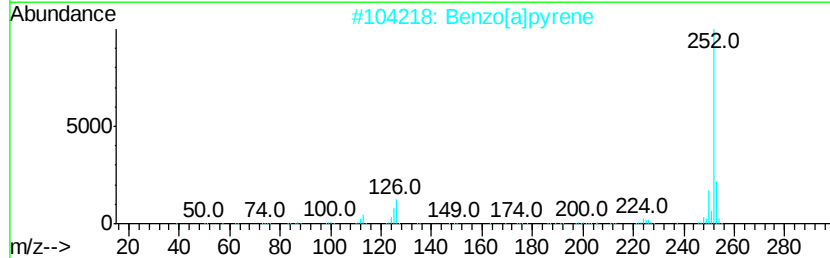
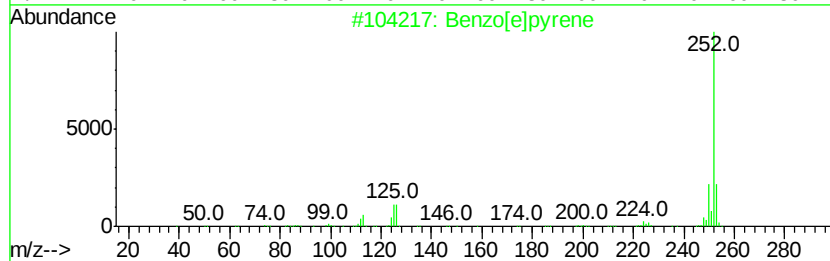
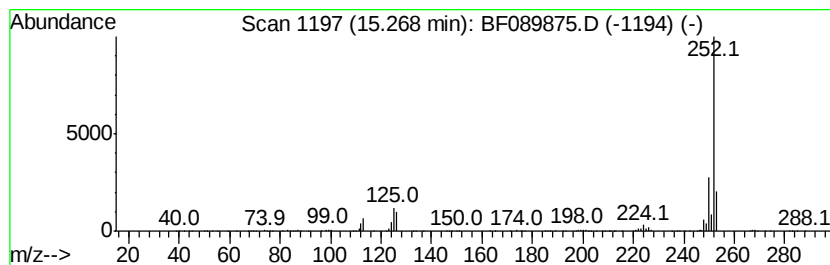
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.69 ng	492369	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[a]pyrene	252	C20H12	000050-32-8	98
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	95
4		Benzo[i]fluoranthene	252	C20H12	000205-82-3	95
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	19.9	ng	2453350	1	6.66	2458950	20.0
unknown6.43	6.43	78.4	ng	9639280	1	6.66	2458950	20.0
Nonadecyl pentafl...	13.75	2.3	ng	631352	5	13.86	5428320	20.0
Benzo[e]pyrene	15.27	3.7	ng	492369	6	15.38	2669870	20.0