

Data Path : V:\HPCHEM1\BNA F\DATA\BF070916\
 Data File : BF088880.D
 Acq On : 9 Jul 2016 19:33
 Operator : UM/SJ
 Sample : H3813-13 25X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS004-0006-01

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-BF063016.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	1.804	17	19	53	rVB	537721	780547	100.00%	16.143%
2	5.187	312	315	320	rBB	8744	9855	1.26%	0.204%
3	5.290	322	324	327	rBV	49970	55112	7.06%	1.140%
4	6.341	415	416	419	rBV	66106	60471	7.75%	1.251%
5	6.479	426	428	430	rBB	79853	62766	8.04%	1.298%
6	6.719	447	449	451	rBB	525487	457685	58.64%	9.466%
7	6.867	460	462	464	rBV	52440	49081	6.29%	1.015%
8	7.279	496	498	500	rBB	43295	39290	5.03%	0.813%
9	7.553	520	522	524	rBB	20772	16623	2.13%	0.344%
10	7.919	553	554	557	rBV	12567	15740	2.02%	0.326%
11	7.999	559	561	564	rBV	574686	559637	71.70%	11.574%
12	8.707	620	623	625	rVB	71948	68494	8.78%	1.417%
13	9.073	653	655	658	rBV	70311	77858	9.97%	1.610%
14	9.702	708	710	712	rVB	13932	12097	1.55%	0.250%
15	9.748	712	714	717	rBV	621662	644402	82.56%	13.327%
16	10.296	758	762	763	rBV3	6317	14342	1.84%	0.297%
17	10.525	781	782	784	rVB	24410	33448	4.29%	0.692%
18	10.833	808	809	811	rBV	11191	8128	1.04%	0.168%
19	10.993	821	823	825	rBV	10511	9404	1.20%	0.194%
20	11.142	834	836	839	rVB2	11026	12807	1.64%	0.265%
21	11.222	841	843	846	rBV2	549641	633396	81.15%	13.100%
22	11.371	855	856	858	rVB	16726	12997	1.67%	0.269%
23	11.462	862	864	868	rBV4	7317	17072	2.19%	0.353%
24	11.542	869	871	873	rVV3	7065	10634	1.36%	0.220%
25	11.679	881	883	886	rBV3	6335	11228	1.44%	0.232%
26	11.759	886	890	891	rBV4	9235	19861	2.54%	0.411%
27	11.885	899	901	902	rVB2	18449	12799	1.64%	0.265%
28	11.965	906	908	911	rVV2	8822	13517	1.73%	0.280%
29	12.274	933	935	936	rBV2	13212	14027	1.80%	0.290%
30	12.434	947	949	951	rBV2	12096	15528	1.99%	0.321%
31	12.811	980	982	984	rBV	74642	88613	11.35%	1.833%
32	13.108	1006	1008	1010	rVB	45169	44669	5.72%	0.924%
33	13.851	1070	1073	1075	rBV	478860	464156	59.47%	9.599%
34	14.239	1105	1107	1109	rVB	72209	59739	7.65%	1.235%

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35	14.502	1128	1130	1132	rBV	99936	145299	18.62%	3.005%
36	15.234	1192	1194	1195	rVB	236765	283902	36.37%	5.872%

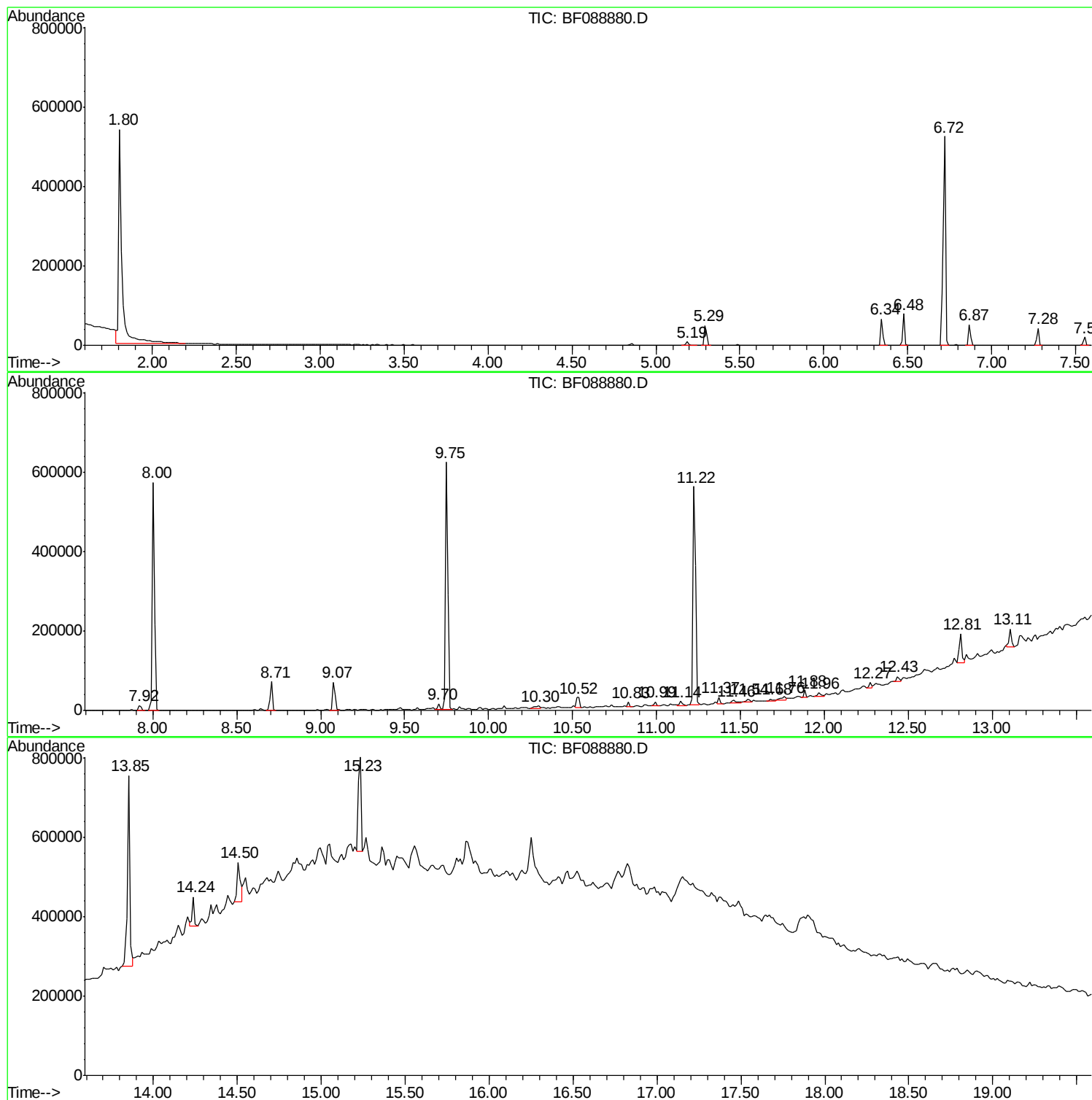
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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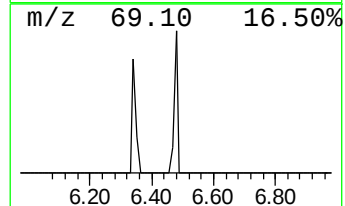
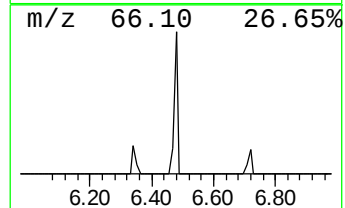
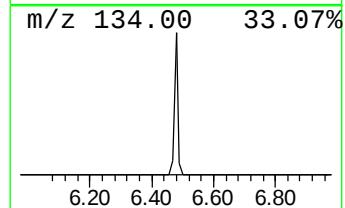
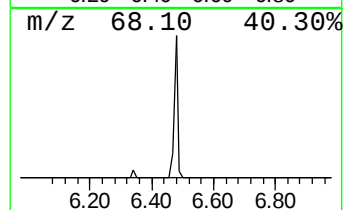
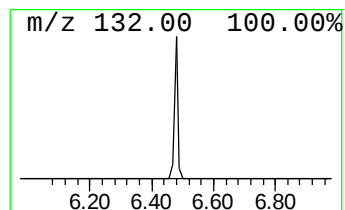
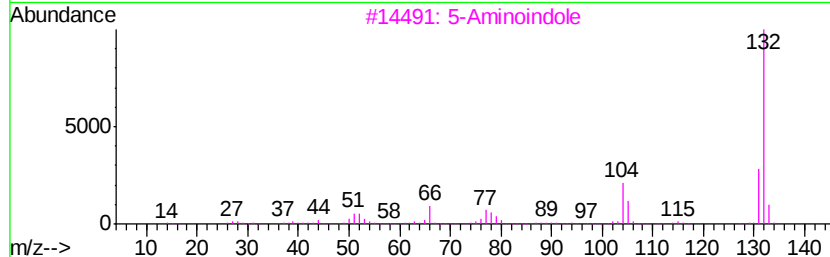
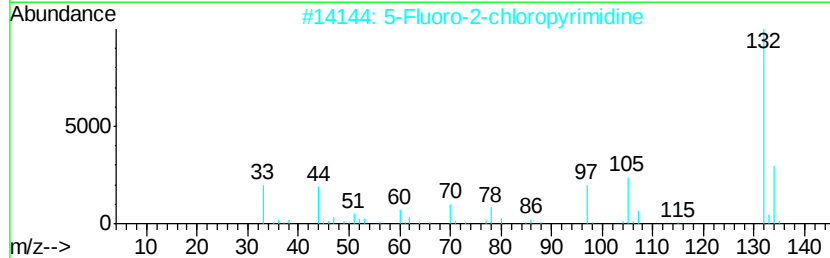
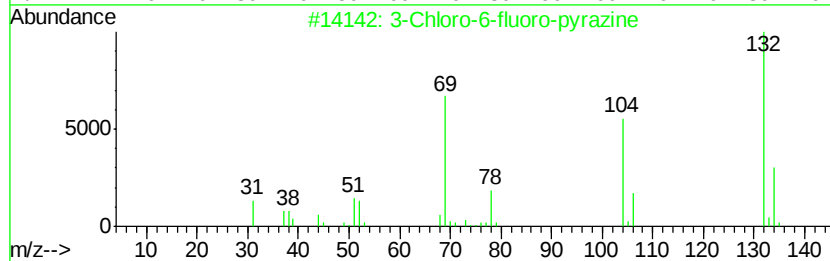
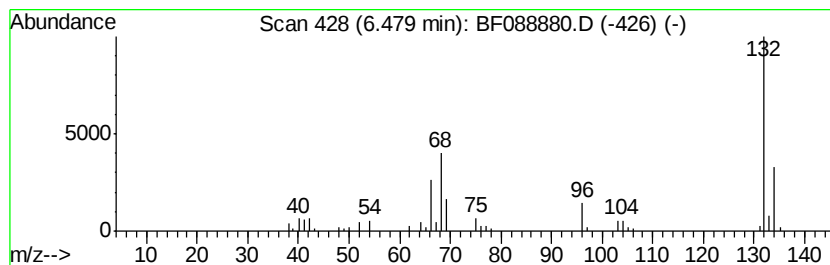
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	2.74 ng	62766	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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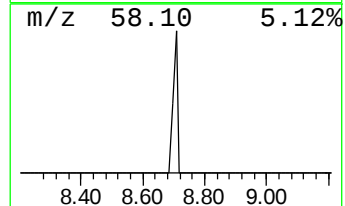
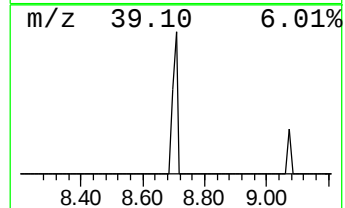
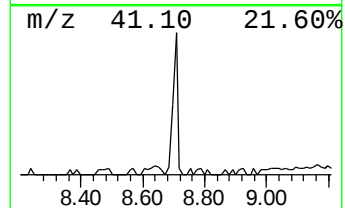
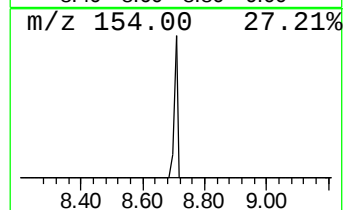
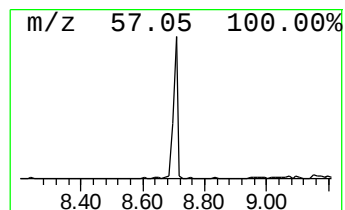
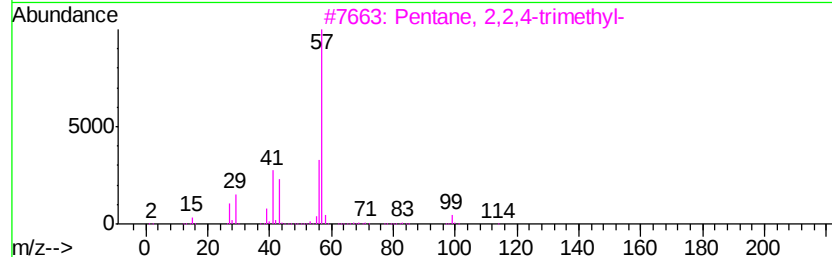
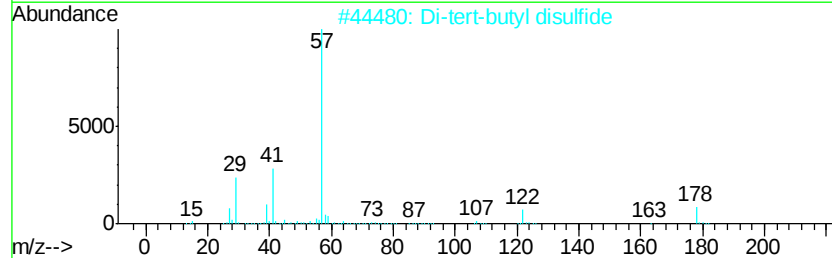
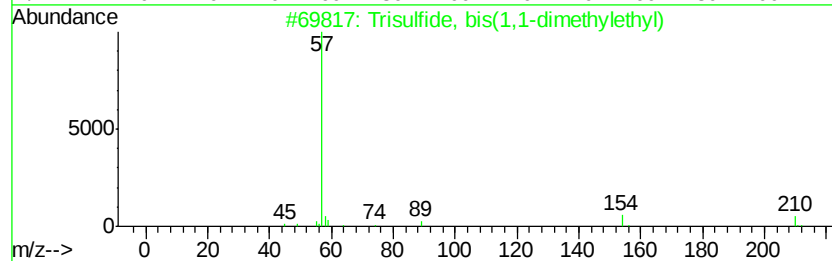
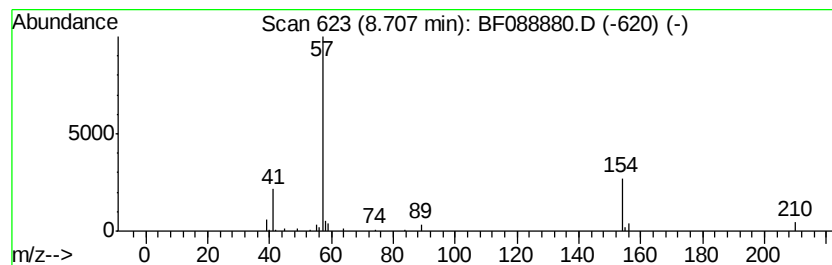
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Peak Number 4 Trisulfide, bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.71	2.45 ng	68494	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	52
2		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	10
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	9
4		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5		di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	9



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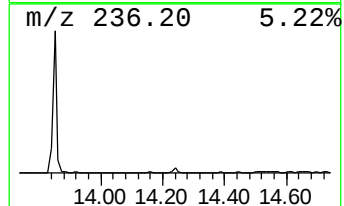
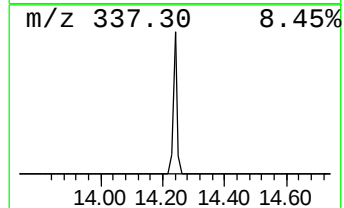
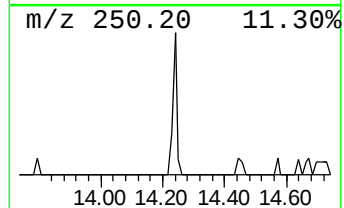
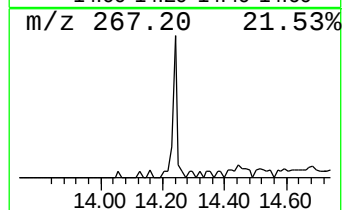
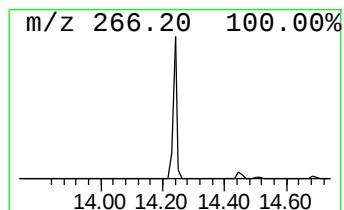
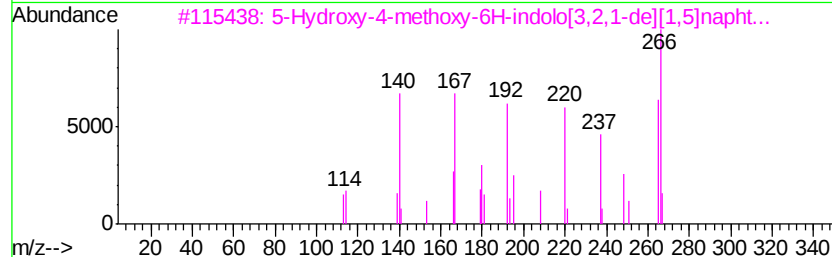
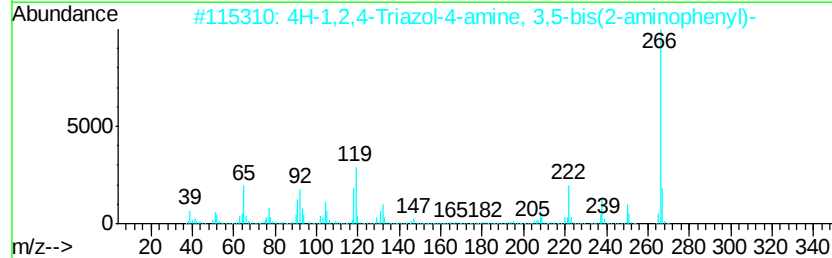
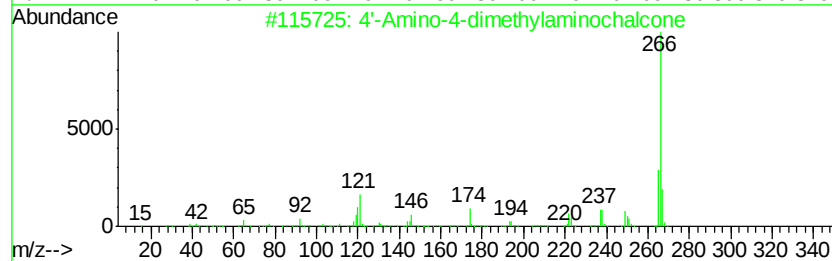
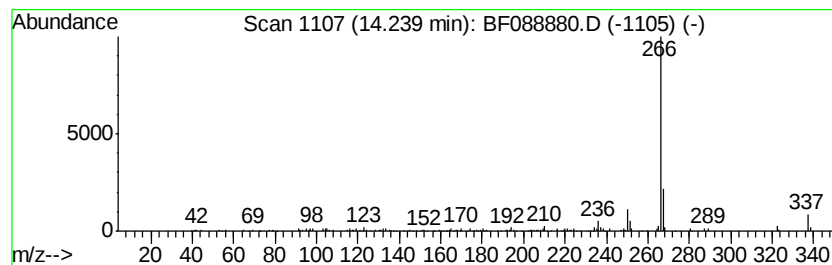
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Peak Number 5 4'-Amino-4-dimethylaminocha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.57 ng	59739	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4'-Amino-4-dimethylaminochalcone	266	C17H18N2O	025870-72-8	72
2		4H-1,2,4-Triazol-4-amine, 3,5-bi...	266	C14H14N6	1000350-00-5	72
3		5-Hydroxy-4-methoxy-6H-indolo[3,...	266	C15H10N2O3	018110-86-6	64
4		Formamide, N-[2-nitrofluoren-9-...	266	C15H10N2O3	027398-54-5	64
5		Perylene, 3-methyl-	266	C21H14	024471-47-4	64



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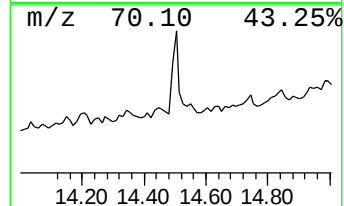
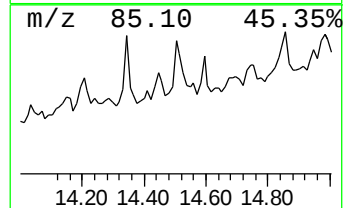
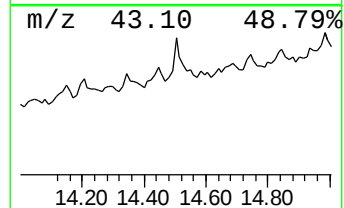
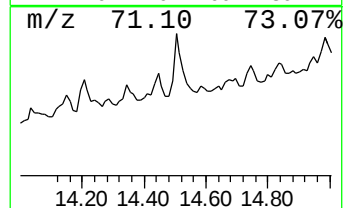
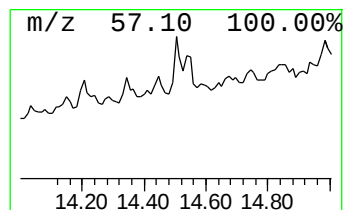
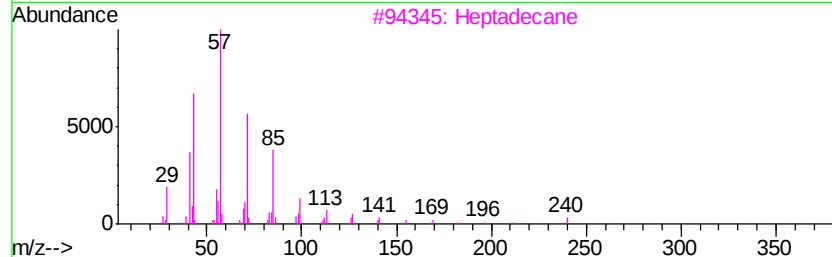
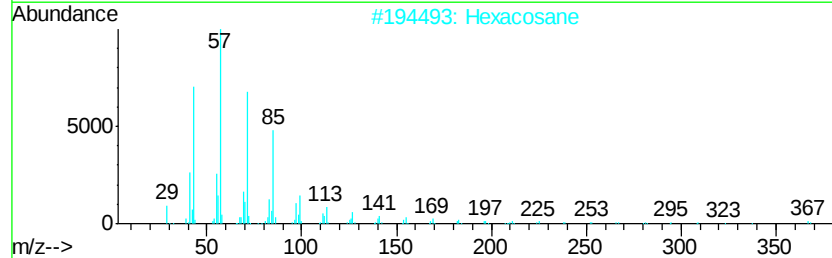
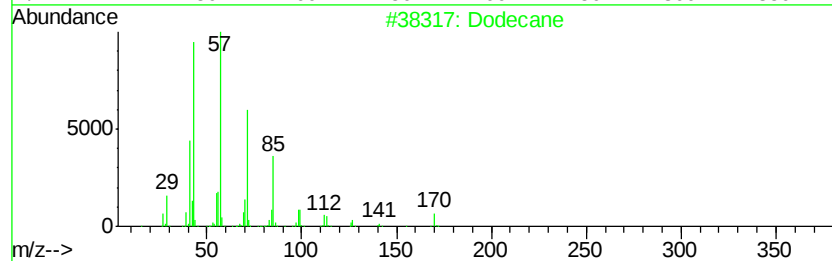
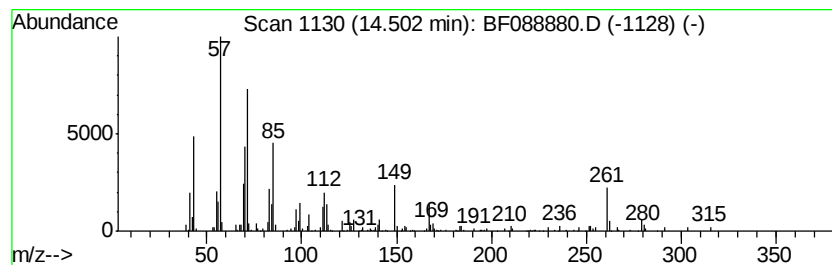
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Peak Number 6 unknown14.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.50	6.26 ng	145299	Chrysene-d12	13.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	46
2	Hexacosane	366	C26H54	000630-01-3	41
3	Heptadecane	240	C17H36	000629-78-7	38
4	Hexadecane	226	C16H34	000544-76-3	38
5	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.48	6.48	2.7	ng	62766	1	6.72	457685	20.0
Trisulfide, bis(1...	8.71	2.5	ng	68494	2	8.00	559637	20.0
4'-Amino-4-dimeth...	14.24	2.6	ng	59739	5	13.85	464156	20.0
unknown14.50	14.50	6.3	ng	145299	5	13.85	464156	20.0