

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041718\
 Data File : BF104569.D
 Acq On : 17 Apr 2018 18:51
 Operator : JU/SJ
 Sample : J2408-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NAA-WS-005

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.022	495	499	507	rBV	125642	166409	4.96%	0.595%
2	5.428	562	568	571	rBV	3006398	3064441	91.38%	10.962%
3	6.069	674	677	681	rBV	33720	40673	1.21%	0.145%
4	6.445	736	741	755	rVB	2814388	3186253	95.01%	11.397%
5	6.575	758	763	766	rBV	3035332	3135940	93.51%	11.217%
6	6.804	798	802	805	rBV	1108263	842284	25.12%	3.013%
7	6.963	824	829	832	rBV	2776894	2478856	73.92%	8.867%
8	7.369	893	898	901	rBV	1932837	1991050	59.37%	7.122%
9	7.457	908	913	924	rVB	42972	56318	1.68%	0.201%
10	8.086	1016	1020	1024	rBV	1304675	1091773	32.56%	3.905%
11	9.163	1198	1203	1207	rBV	3425919	3353557	100.00%	11.996%
12	9.557	1266	1270	1273	rBV	489168	377185	11.25%	1.349%
13	9.769	1302	1306	1310	rVB	81966	58857	1.76%	0.211%
14	9.845	1315	1319	1323	rVV	1284214	1098746	32.76%	3.930%
15	10.245	1384	1387	1389	rBV	33470	34201	1.02%	0.122%
16	10.269	1389	1391	1394	rVB	120151	83407	2.49%	0.298%
17	10.486	1423	1428	1431	rBV	28093	36162	1.08%	0.129%
18	10.633	1449	1453	1463	rVB	1792598	1700851	50.72%	6.084%
19	10.739	1469	1471	1481	rBV	89232	99190	2.96%	0.355%
20	11.192	1545	1548	1550	rBV	53467	41266	1.23%	0.148%
21	11.333	1568	1572	1575	rBV	1040155	903634	26.95%	3.232%
22	12.921	1837	1842	1845	rBV	2626574	2436220	72.65%	8.714%
23	13.780	1982	1988	1990	rBV	63838	94826	2.83%	0.339%
24	13.810	1990	1993	2001	rVB	118550	129640	3.87%	0.464%
25	13.974	2017	2021	2025	rBV	921754	832113	24.81%	2.977%
26	15.439	2265	2270	2279	rBV	483496	622090	18.55%	2.225%

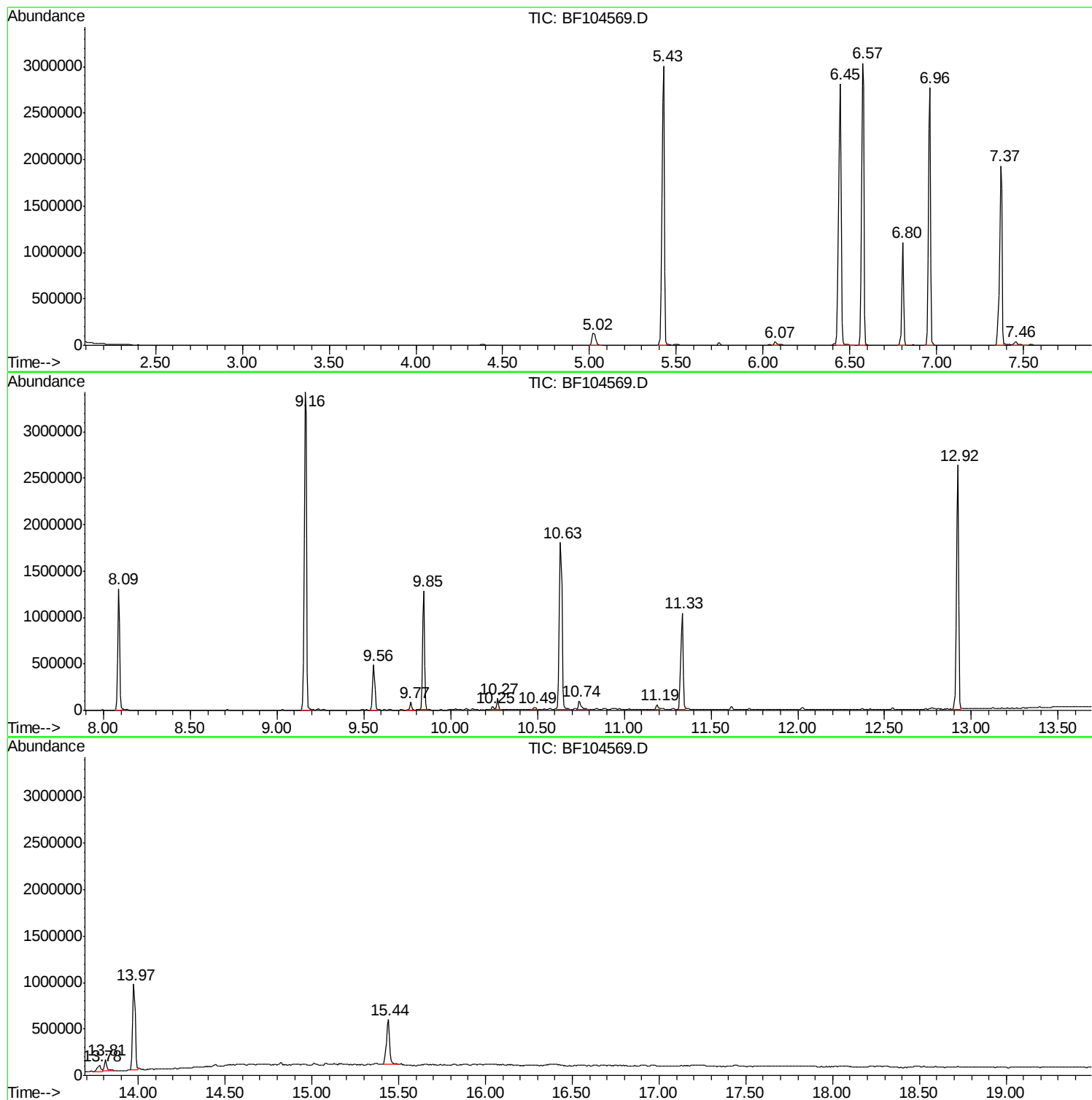
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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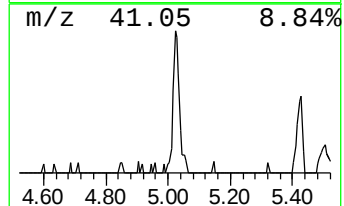
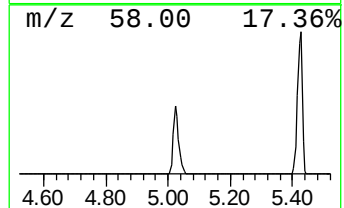
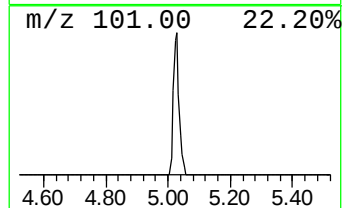
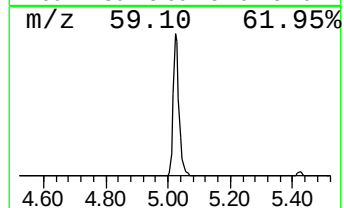
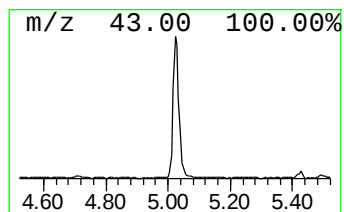
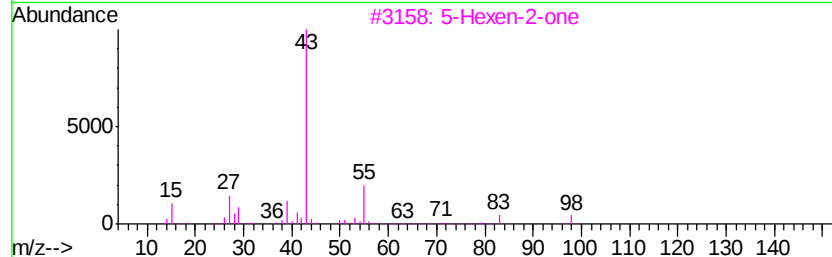
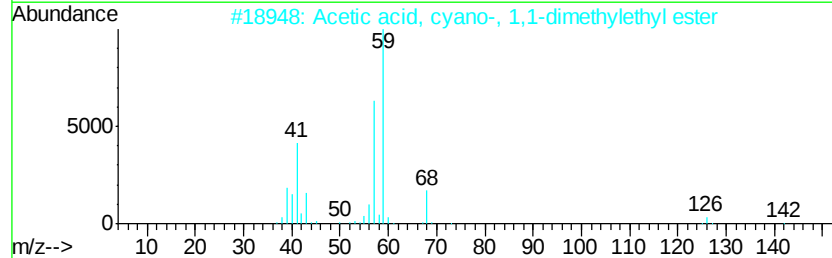
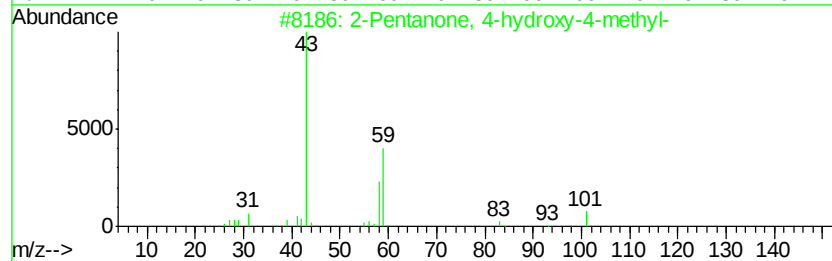
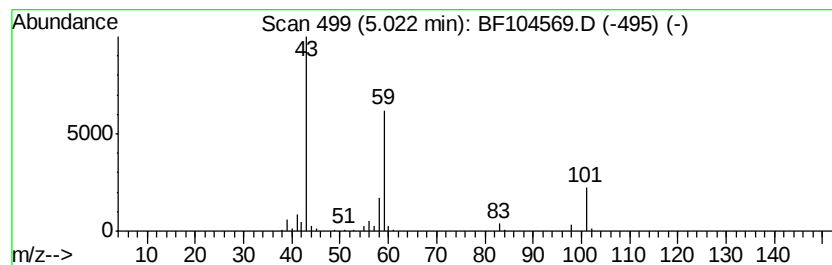
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.95 ng	166409	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	17
3	5-Hexen-2-one	98	C6H10O		000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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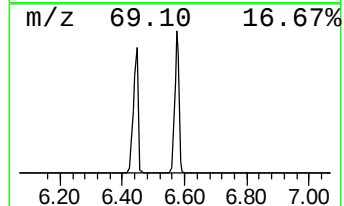
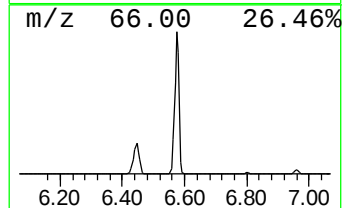
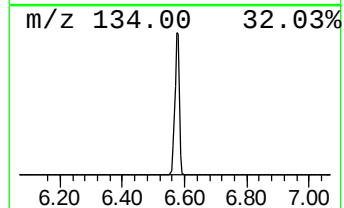
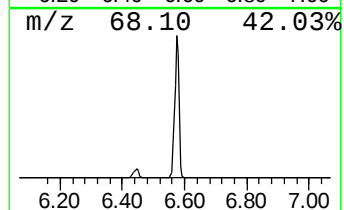
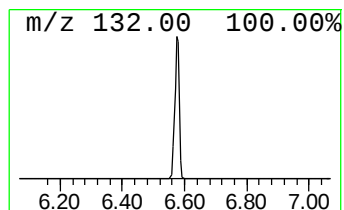
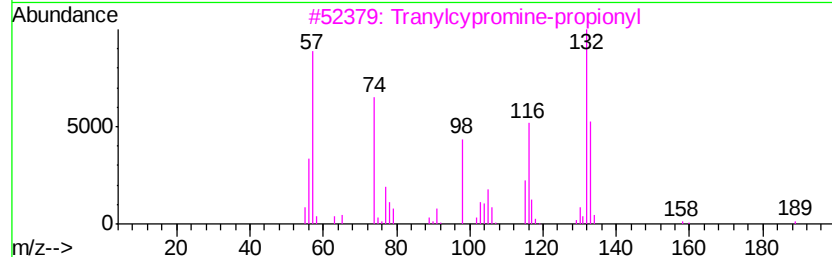
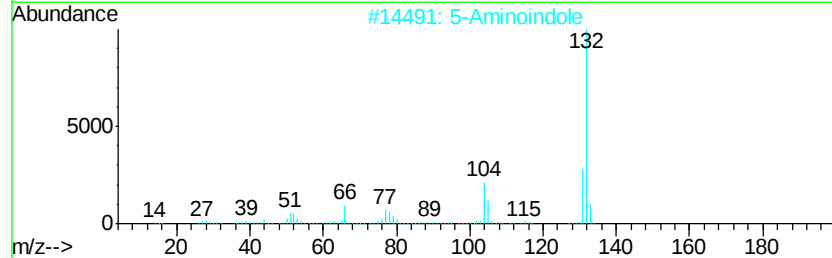
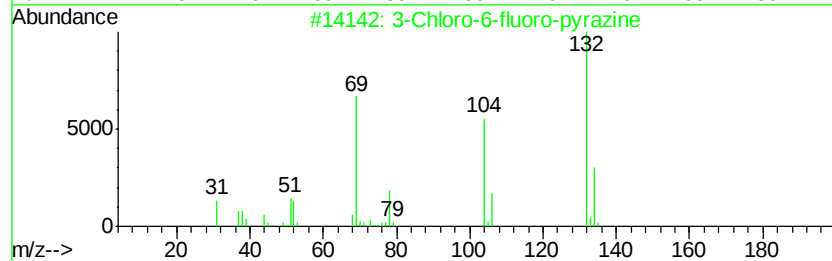
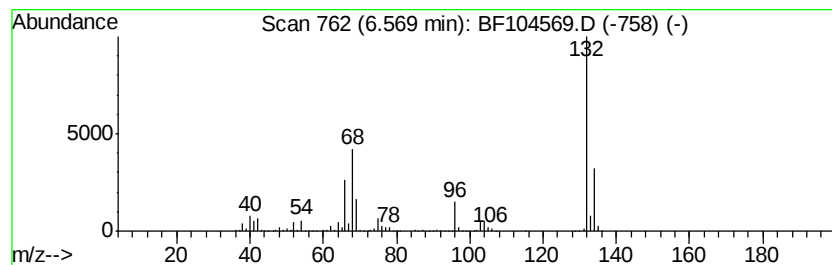
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	74.46 ng	3135940	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9



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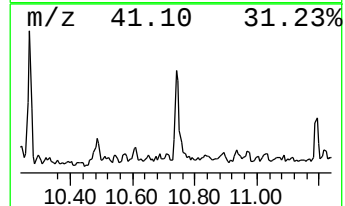
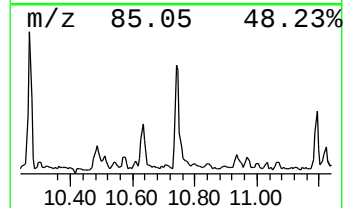
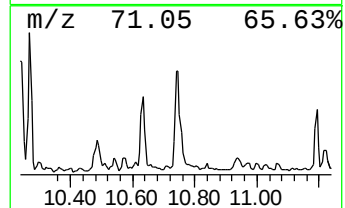
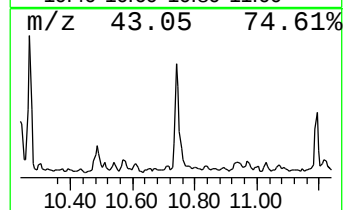
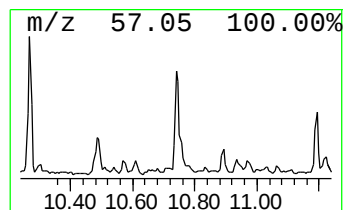
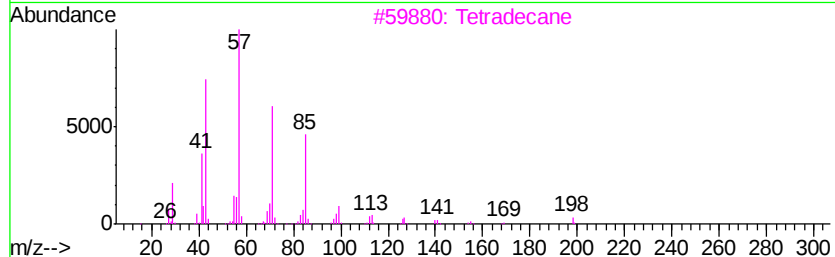
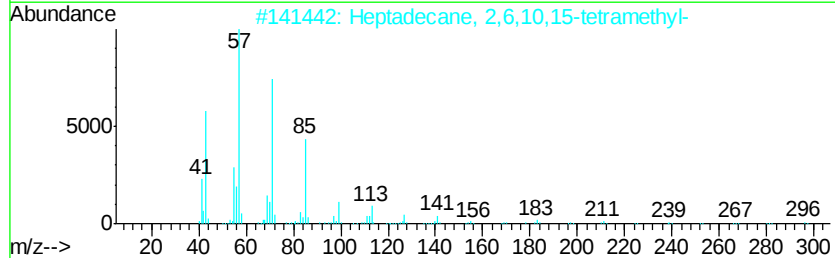
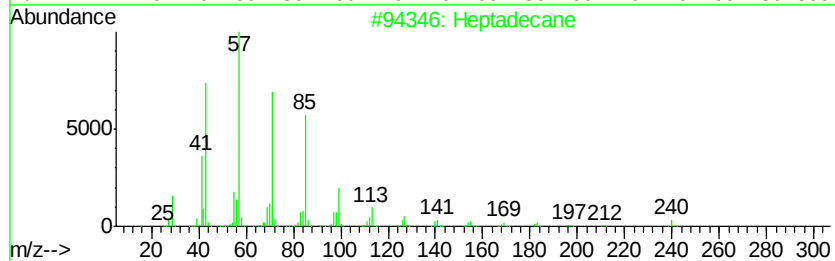
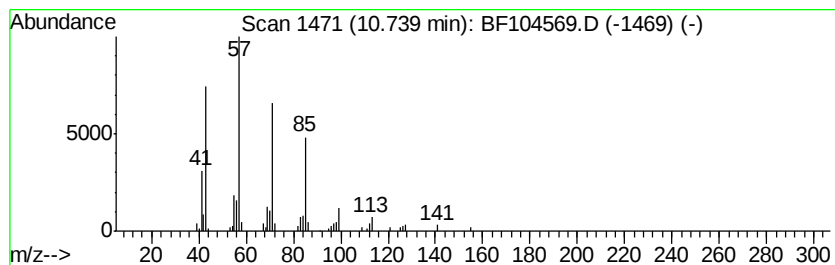
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Peak Number 4 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.20 ng	99190	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	87
3	Tetradecane		198	C14H30	000629-59-4	87
4	Decane, 2,4,6-trimethyl-		184	C13H28	062108-27-4	86
5	Sulfurous acid, 2-propyl tetra...		320	C17H36O3S	1000309-12-5	86



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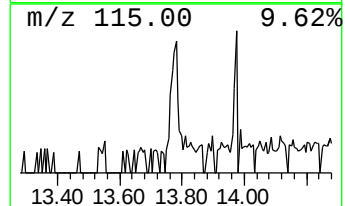
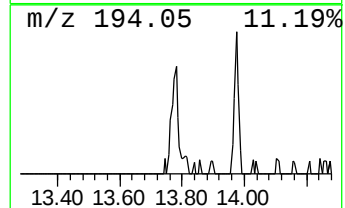
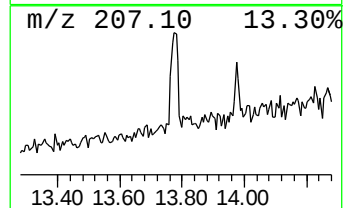
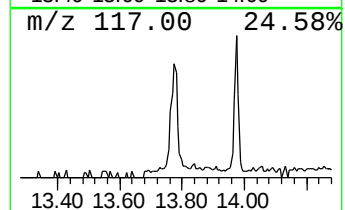
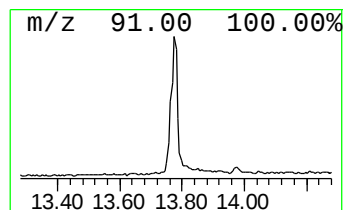
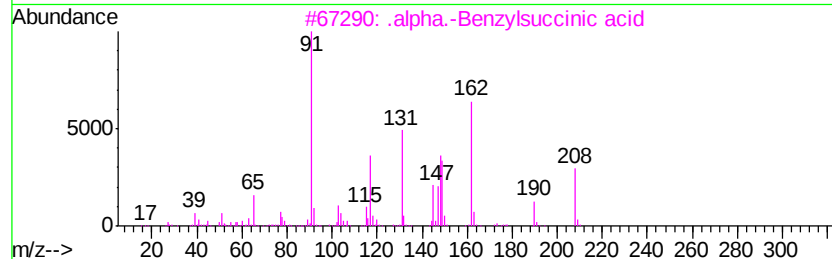
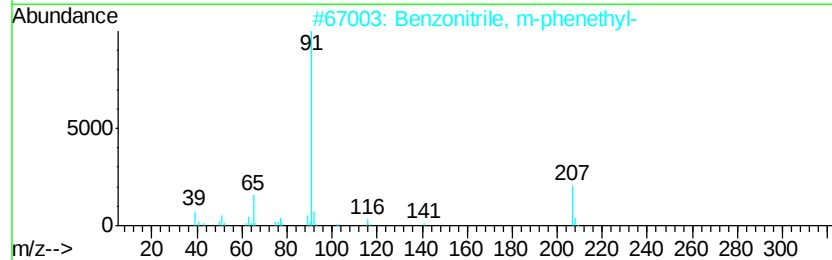
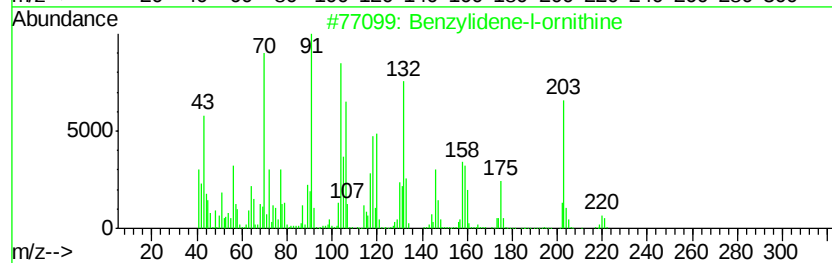
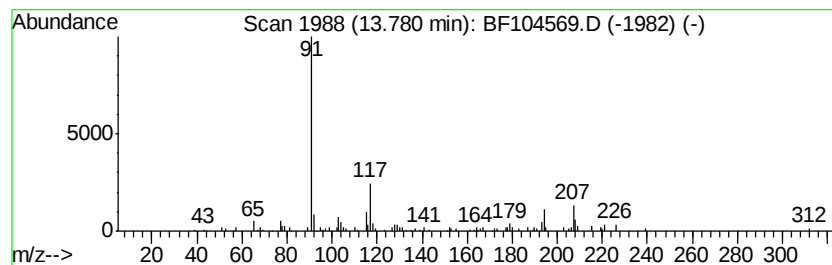
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Peak Number 5 unknown13.78 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.28 ng	94826	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzylidene-L-ornithine	220	C12H16N2O2	025693-00-9	35
2		Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	16
3		.alpha.-Benzylsuccinic acid	208	C11H12O4	000884-33-3	16
4		2,3-Butanediol, 1,4-bis[(benzylol...	388	C20H24N2O6	1000163-34-1	12
5		2,5-Diphenyltetrazole	222	C13H10N4	018039-45-7	12



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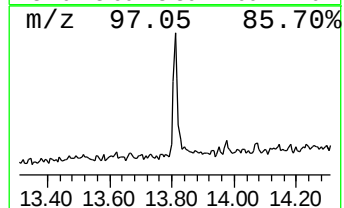
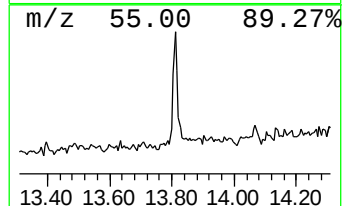
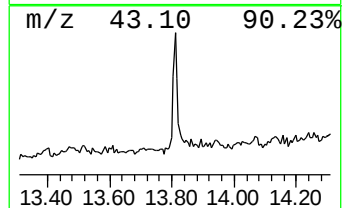
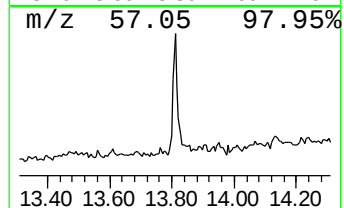
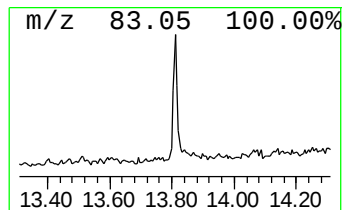
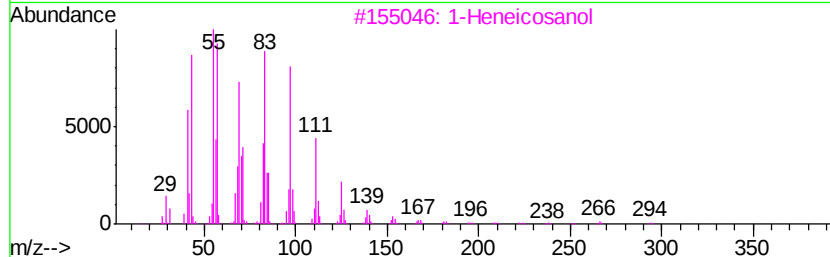
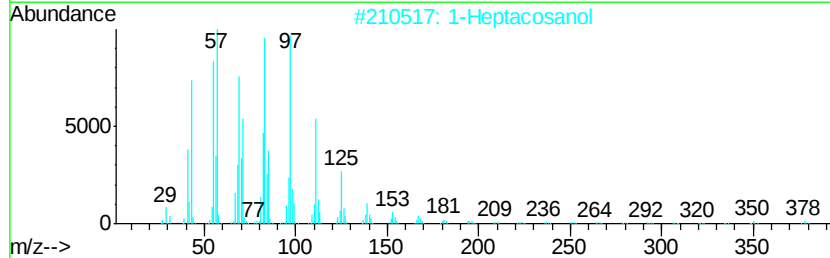
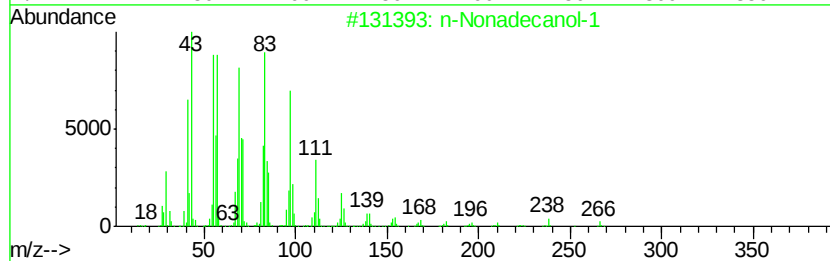
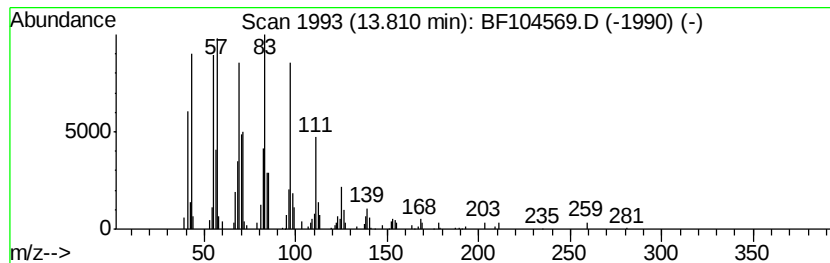
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.12 ng	129640	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		1-Octadecanol	270	C18H38O	000112-92-5	95
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	4.0	ng	166409	1	6.80	842284	20.0
unknown6.57	6.57	74.5	ng	3135940	1	6.80	842284	20.0
Heptadecane	10.74	2.2	ng	99190	4	11.33	903634	20.0
unknown13.78	13.78	2.3	ng	94826	5	13.97	832113	20.0
n-Nonadecanol-1	13.81	3.1	ng	129640	5	13.97	832113	20.0