

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031117\
 Data File : BF093601.D
 Acq On : 12 Mar 2017 9:55
 Operator : SJ/MA
 Sample : I2198-02
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-23

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-BF030717.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	4.870	259	261	270	rBV	102785	215286	4.20%	0.683%
2	5.316	298	300	320	rBV	1566584	2145055	41.84%	6.810%
3	6.379	391	393	401	rBV	980872	1539918	30.04%	4.889%
4	6.493	401	403	415	rVB	3893745	3863539	75.37%	12.265%
5	6.722	421	423	425	rBV	920967	1004785	19.60%	3.190%
6	6.870	434	436	439	rBV	3135233	3514693	68.56%	11.158%
7	7.293	471	473	476	rBV	2450480	2838750	55.38%	9.012%
8	8.013	533	536	538	rBV	927226	1315357	25.66%	4.176%
9	9.088	627	630	632	rBV	5197667	5126331	100.00%	16.274%
10	9.488	663	665	670	rVB	110786	100127	1.95%	0.318%
11	9.762	686	689	691	rBV	1091248	1318534	25.72%	4.186%
12	10.551	755	758	761	rBV	1965937	1974235	38.51%	6.268%
13	10.665	766	768	775	rVB2	59210	108125	2.11%	0.343%
14	11.111	805	807	808	rBV	41479	56814	1.11%	0.180%
15	11.248	816	819	821	rBV	880823	1055973	20.60%	3.352%
16	12.722	945	948	954	rBV	79745	108434	2.12%	0.344%
17	12.825	954	957	959	rBV	3466903	3292226	64.22%	10.452%
18	13.728	1033	1036	1039	rBV2	58114	98421	1.92%	0.312%
19	13.877	1047	1049	1052	rBV	904593	955819	18.65%	3.034%
20	15.283	1169	1172	1176	rBV	579016	867030	16.91%	2.753%

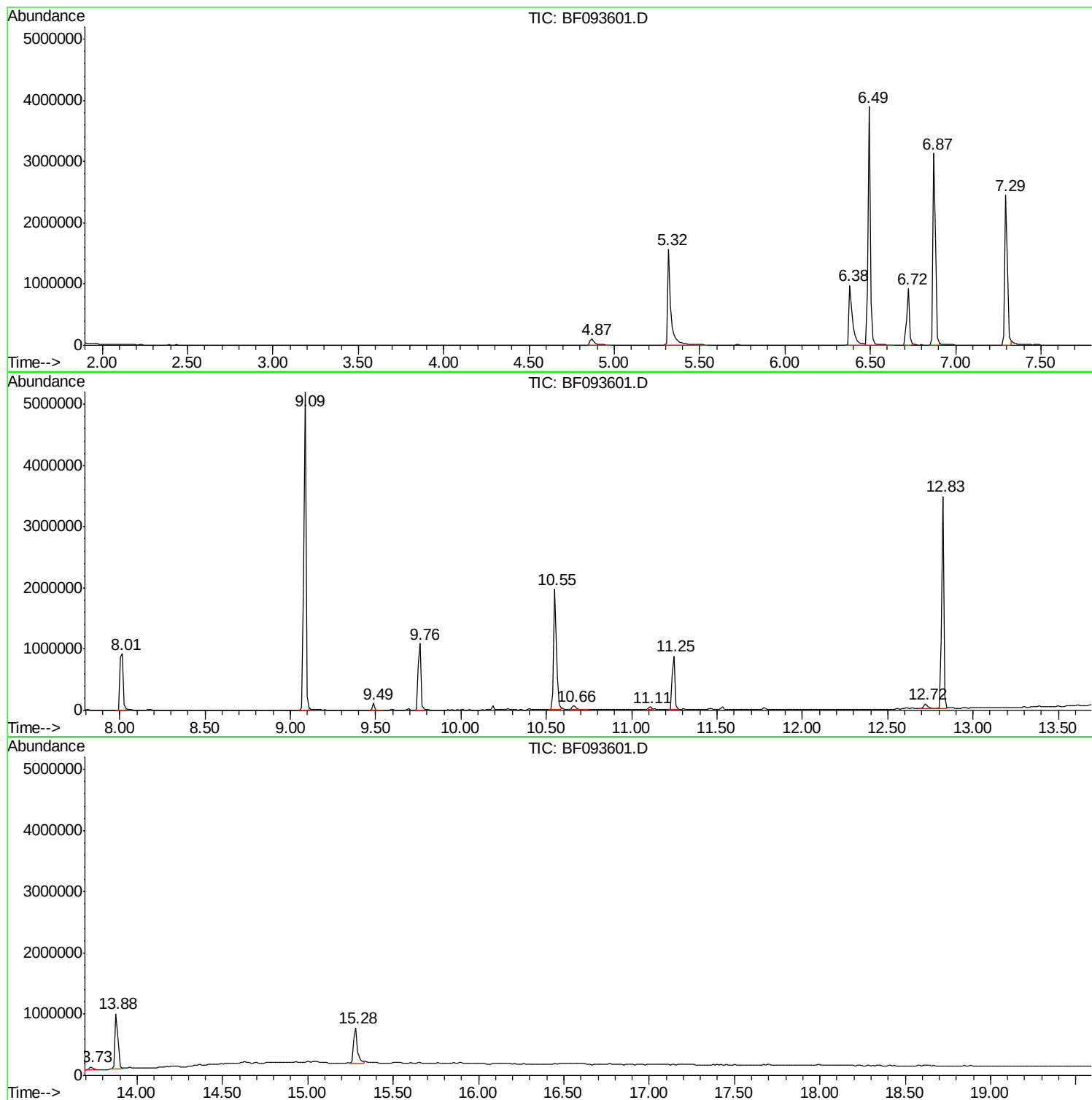
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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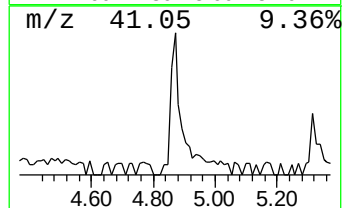
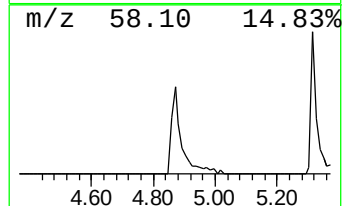
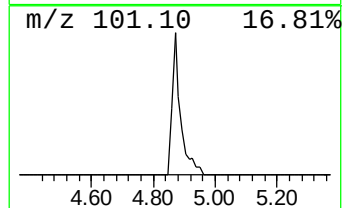
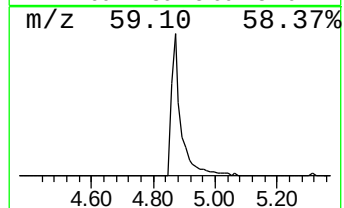
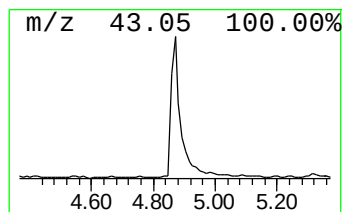
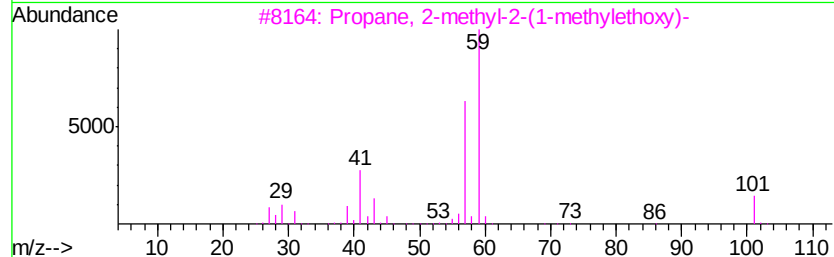
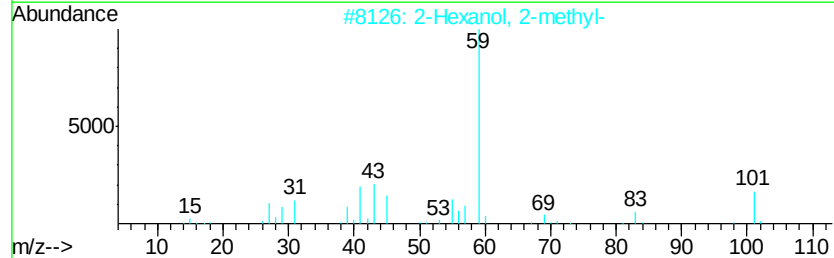
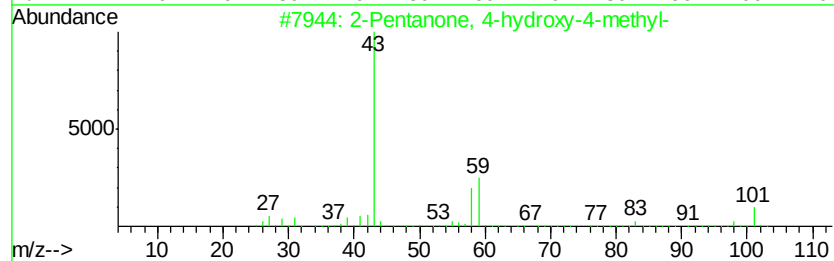
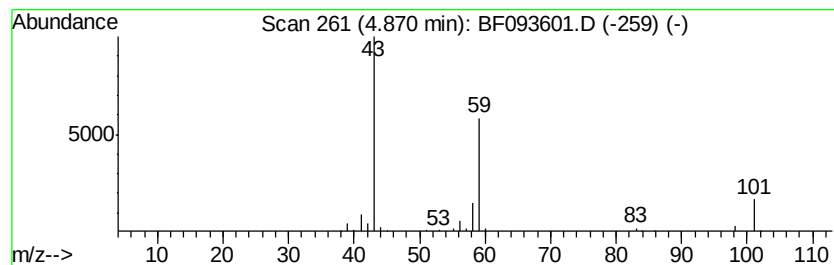
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	4.29 ng	215286	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33



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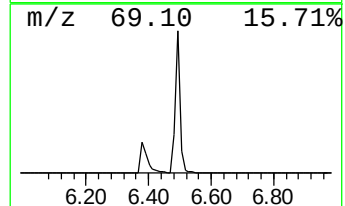
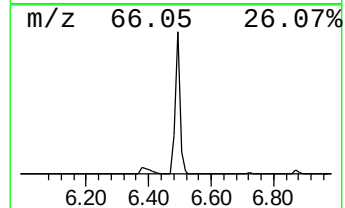
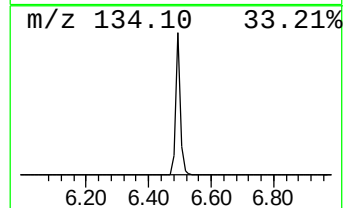
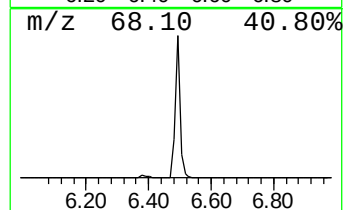
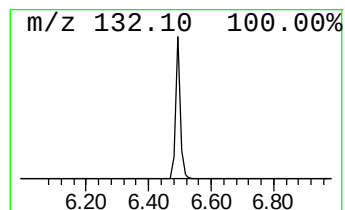
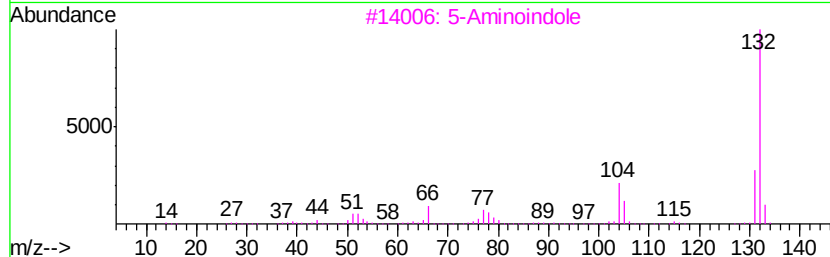
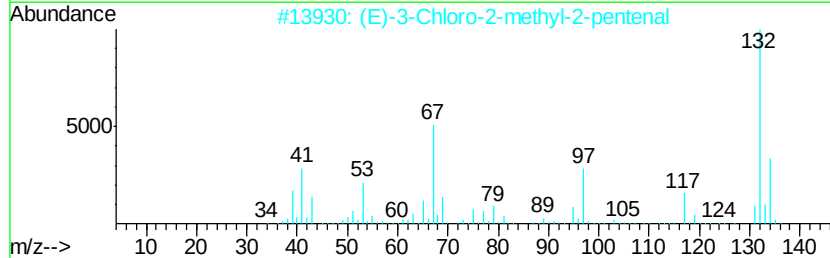
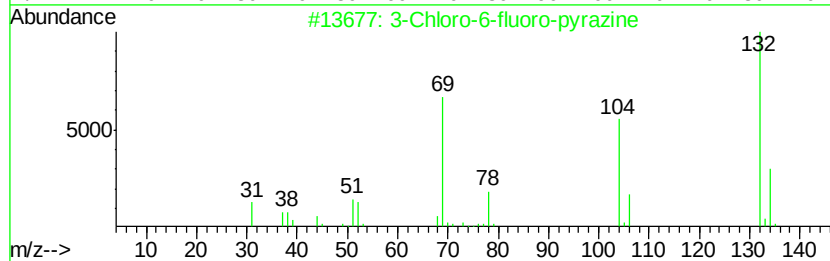
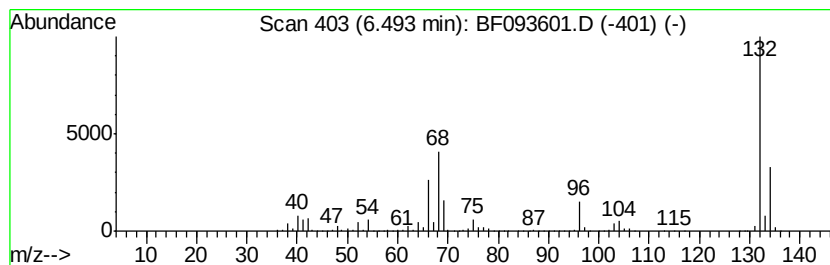
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	76.90 ng	3863540	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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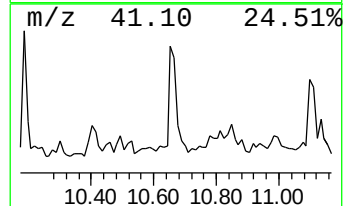
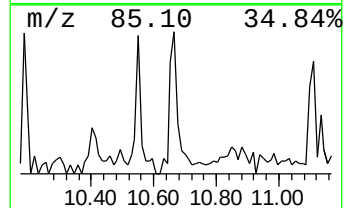
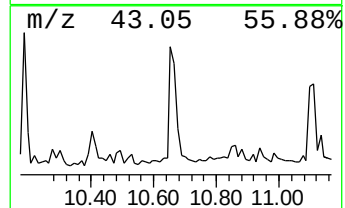
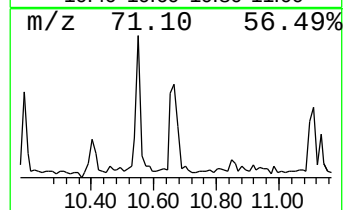
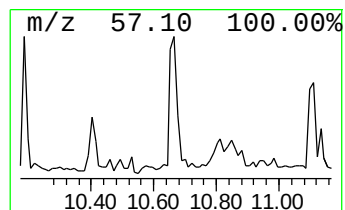
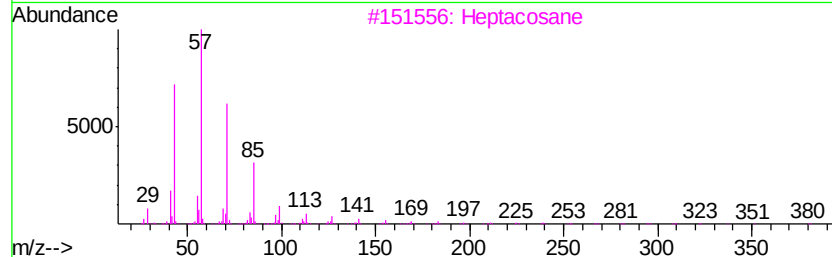
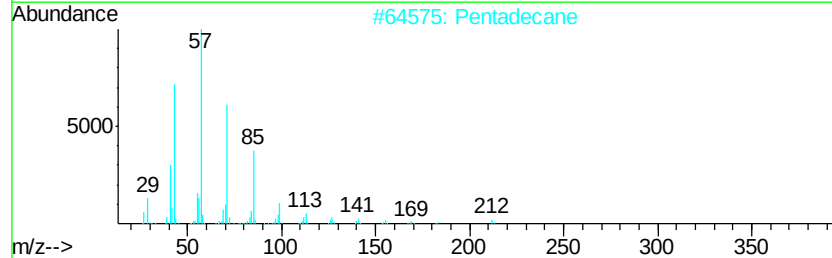
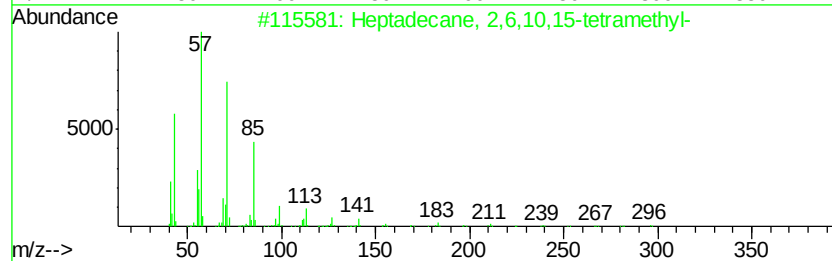
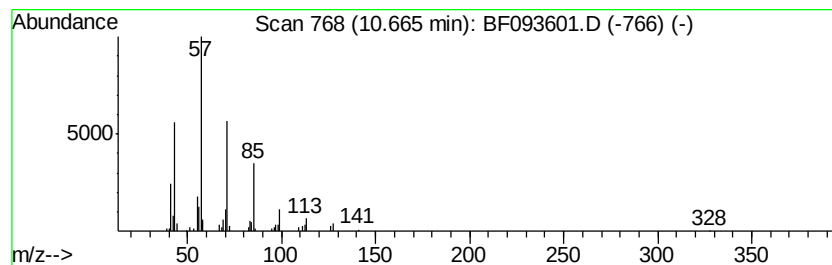
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Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.05 ng	108125	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane,	2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Pentadecane		212	C15H32	000629-62-9	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Tetradecane		198	C14H30	000629-59-4	86



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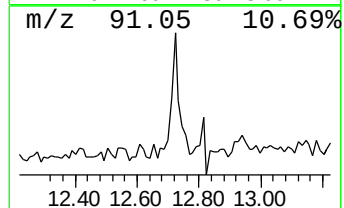
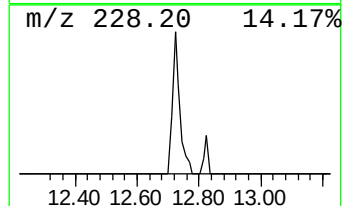
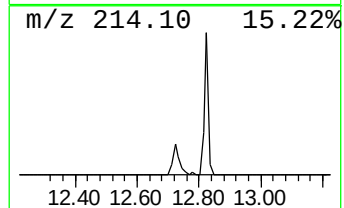
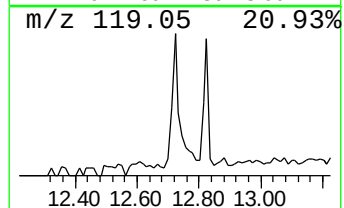
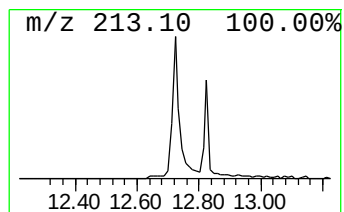
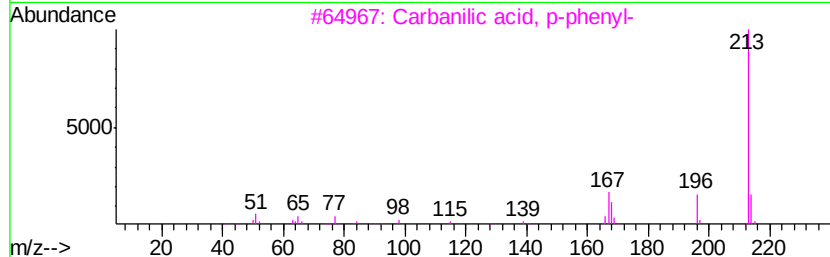
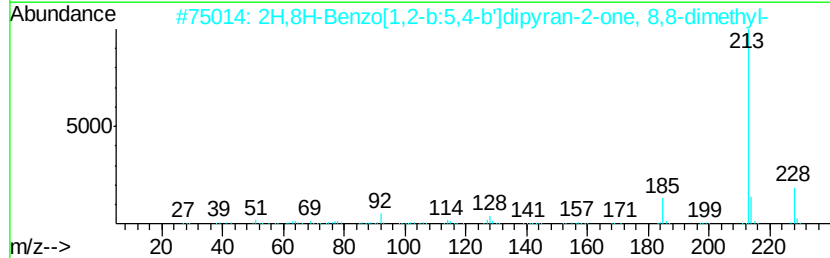
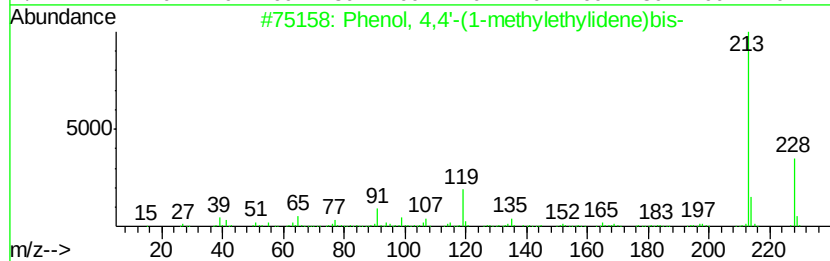
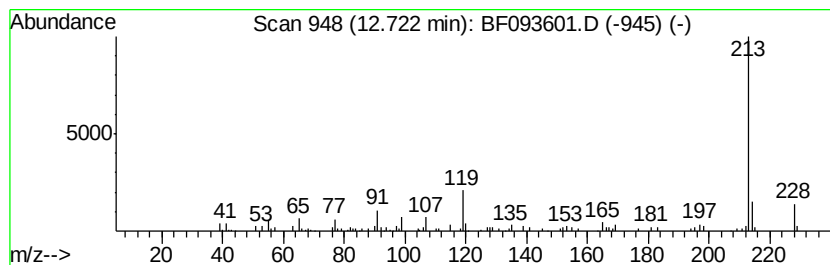
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Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.27 ng	108434	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	94	
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53	
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50	
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	47	
5	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40	



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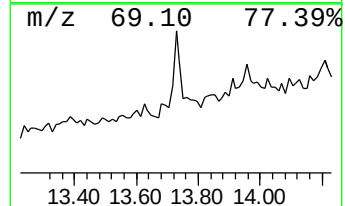
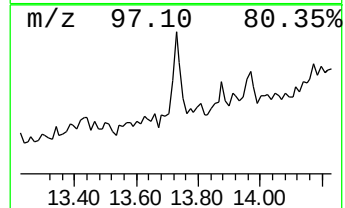
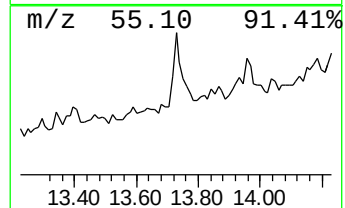
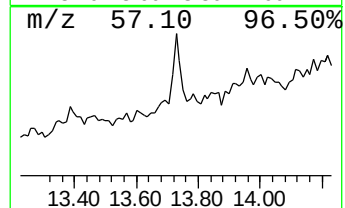
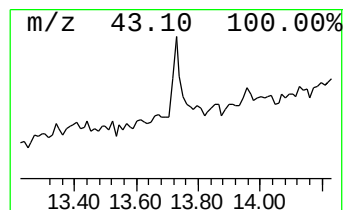
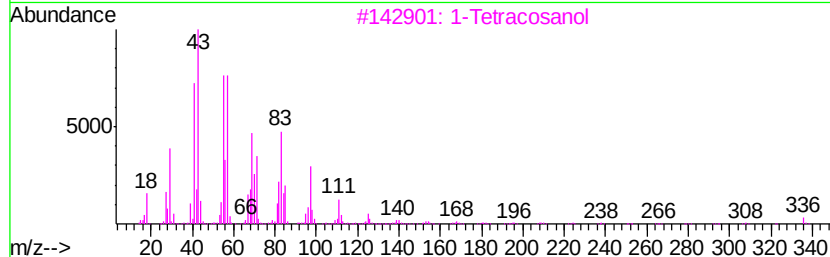
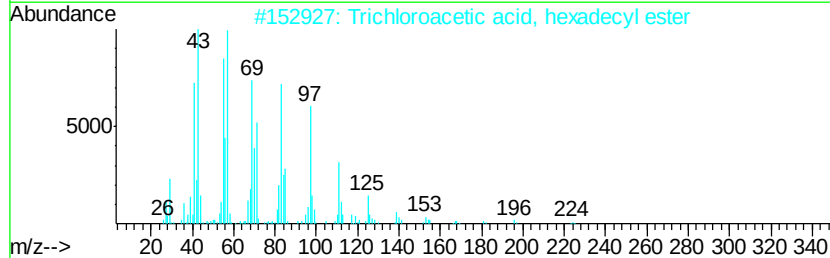
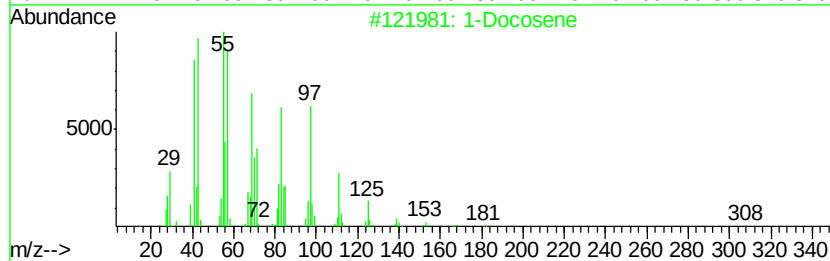
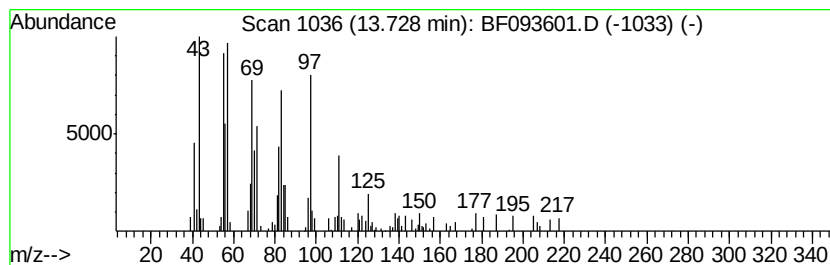
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	2.06 ng	98421	Chrysene-d12	13.88	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	68
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
3	1-Tetracosanol	354	C24H50O	000506-51-4	62
4	1-Octadecene	252	C18H36	000112-88-9	58
5	Cyclopentadecane	210	C15H30	000295-48-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	4.3	ng	215286	1	6.72	1004790	20.0
unknown6.49	6.49	76.9	ng	3863540	1	6.72	1004790	20.0
Heptadecane, 2,6,...	10.67	2.0	ng	108125	4	11.25	1055970	20.0
Phenol, 4,4'-(1-m...	12.72	2.3	ng	108434	5	13.88	955819	20.0
1-Docosene	13.73	2.1	ng	98421	5	13.88	955819	20.0