

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092616\
 Data File : BF090240.D
 Acq On : 27 Sep 2016 1:40
 Operator : UM/SJ
 Sample : H4946-11
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-06D-092216

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-BF092016.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	1.656	4	6	13	rBV	3076625	7491683	100.00%	23.011%
2	1.781	14	17	61	rVB	1906427	4134696	55.19%	12.700%
3	4.547	257	259	264	rBV	132127	185574	2.48%	0.570%
4	5.027	299	301	304	rBV	756500	1121791	14.97%	3.446%
5	6.125	395	397	405	rBV	671523	773751	10.33%	2.377%
6	6.239	405	407	410	rBV	1856847	2038508	27.21%	6.261%
7	6.479	426	428	430	rBV	914889	833589	11.13%	2.560%
8	6.639	439	442	444	rBV	1779329	2150119	28.70%	6.604%
9	7.050	475	478	481	rBV	1575192	1589641	21.22%	4.883%
10	7.770	538	541	543	rBV	1081132	1119082	14.94%	3.437%
11	8.525	603	607	609	rBV	249463	411135	5.49%	1.263%
12	8.845	633	635	638	rBV	2565981	2881123	38.46%	8.850%
13	9.245	668	670	677	rVB	136365	125994	1.68%	0.387%
14	9.508	691	693	695	rBV	1459056	1219812	16.28%	3.747%
15	10.296	759	762	764	rBV	1352587	1596531	21.31%	4.904%
16	10.982	819	822	824	rBV	779940	1015419	13.55%	3.119%
17	12.559	957	960	963	rBV	2137627	2110768	28.17%	6.483%
18	13.474	1032	1040	1045	rBV2	45243	83839	1.12%	0.258%
19	13.588	1048	1050	1052	rBV	815394	824878	11.01%	2.534%
20	13.908	1070	1078	1085	rBV8	24651	128127	1.71%	0.394%
21	14.914	1163	1166	1168	rBV	521034	720600	9.62%	2.213%

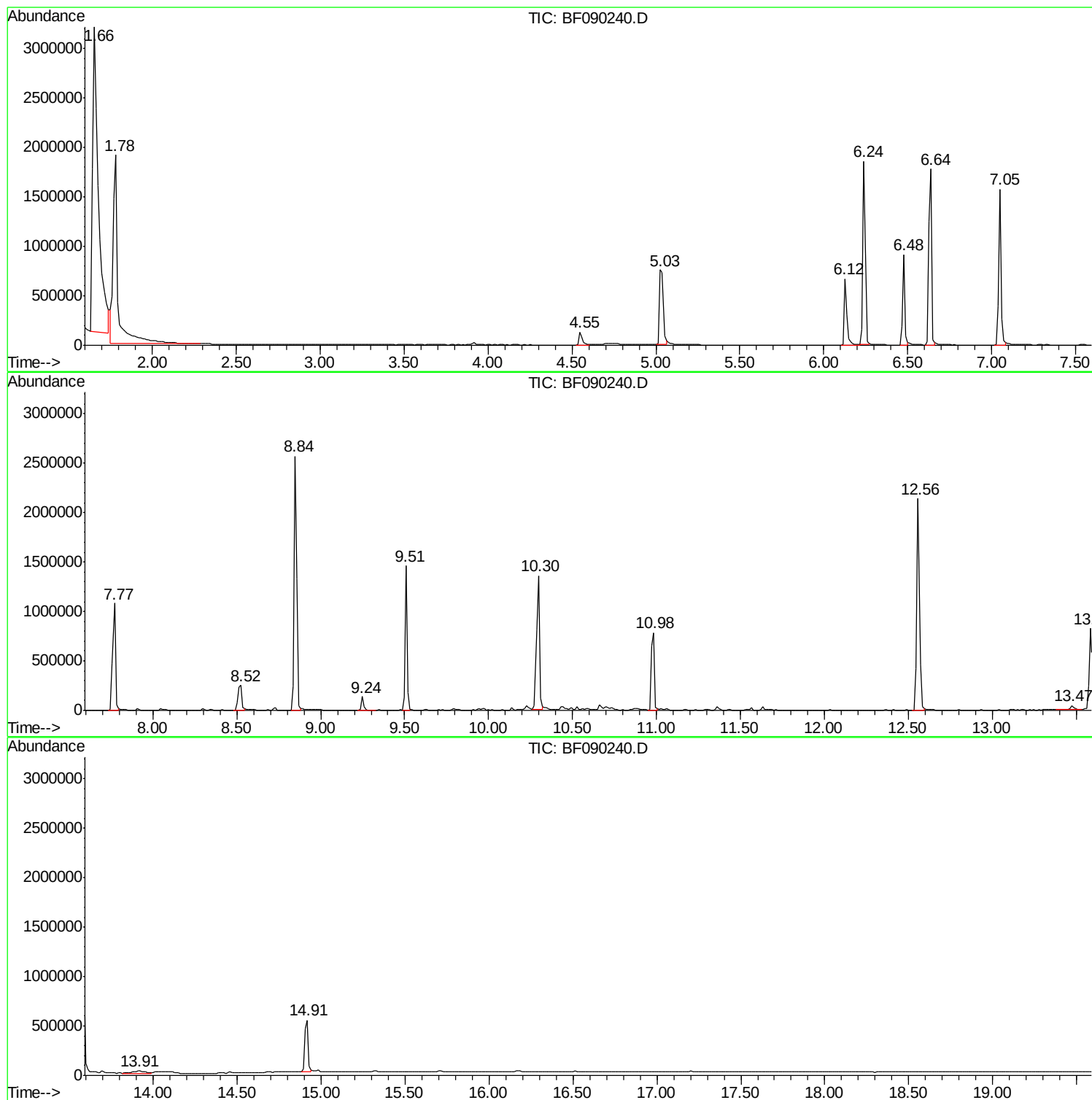
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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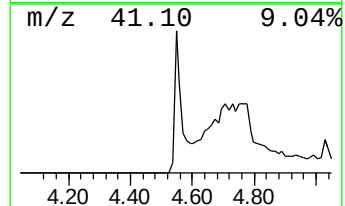
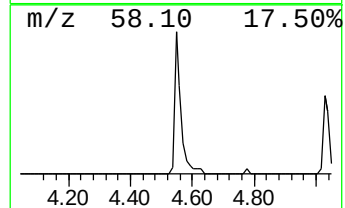
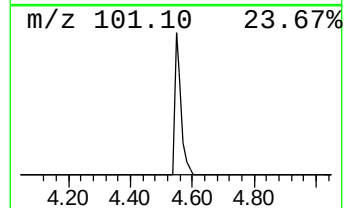
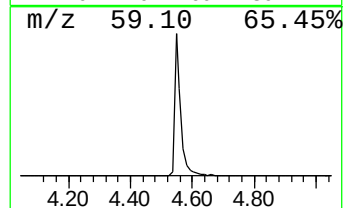
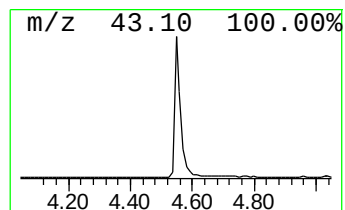
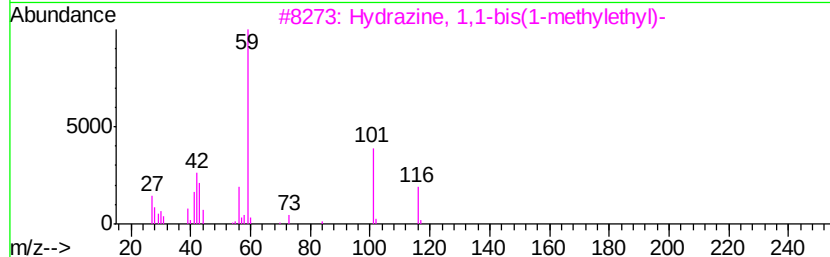
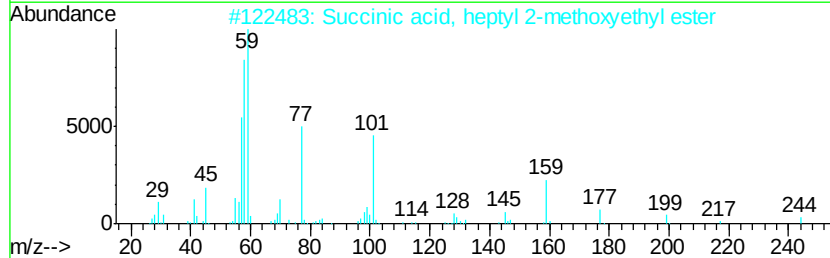
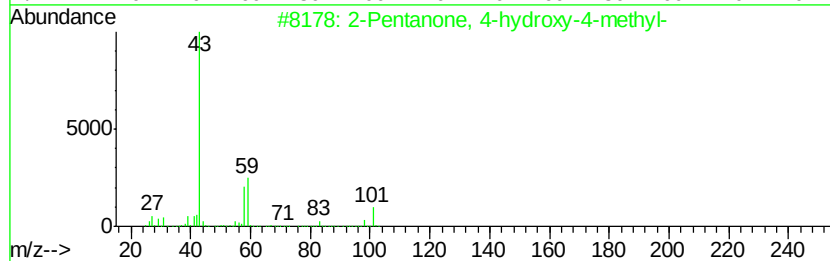
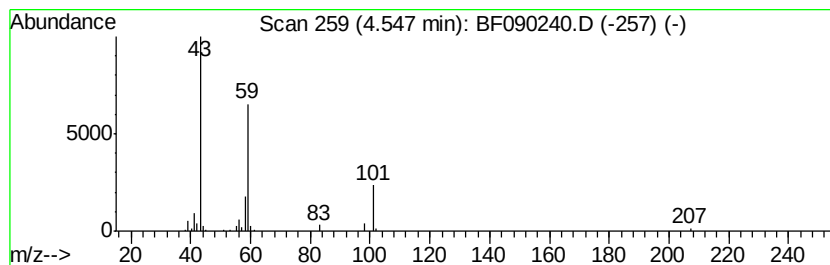
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	4.45 ng	185574	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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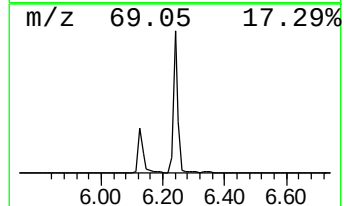
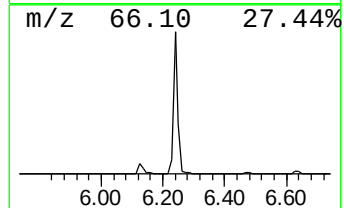
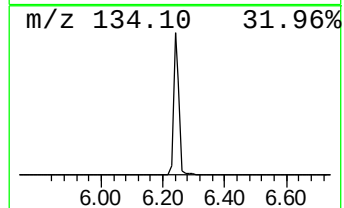
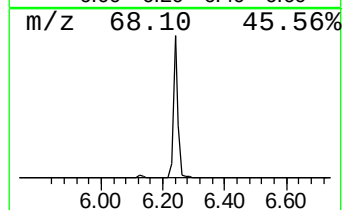
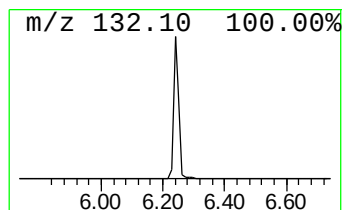
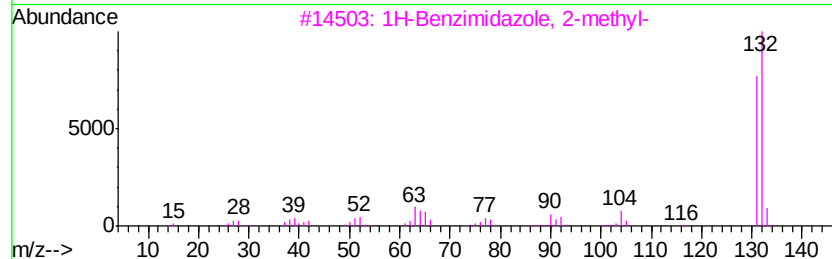
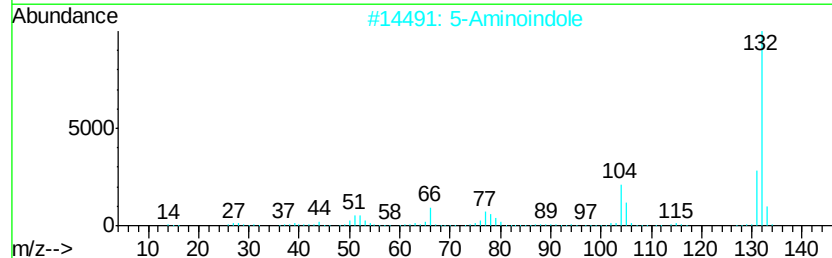
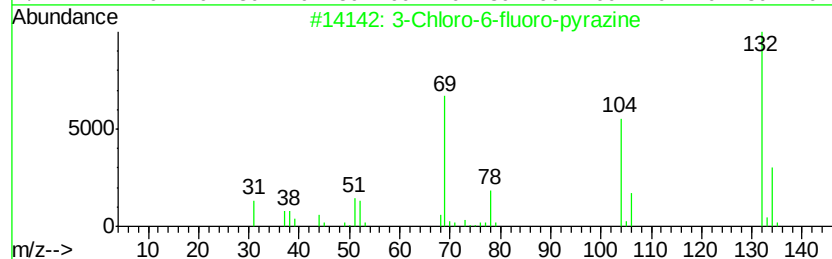
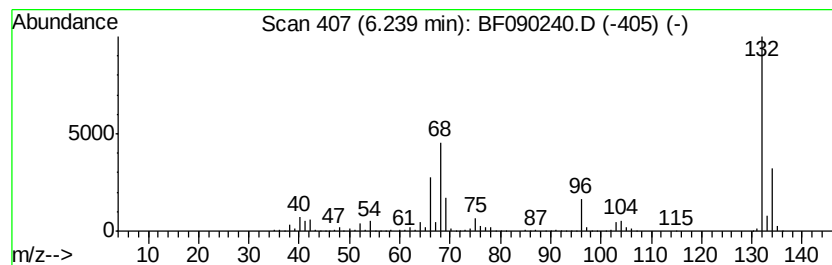
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Peak Number 4 unknown6.24 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	48.91 ng	2038510	1,4-Dichlorobenzene-d4	6.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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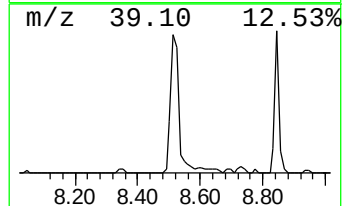
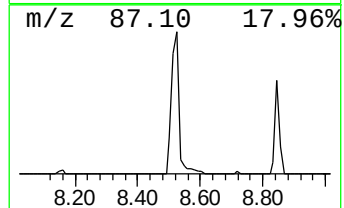
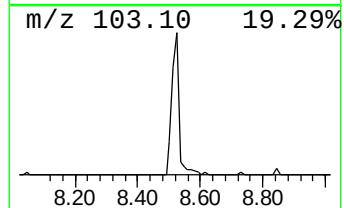
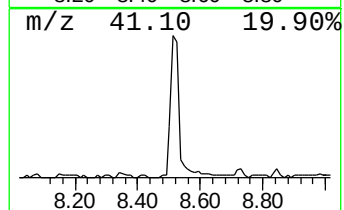
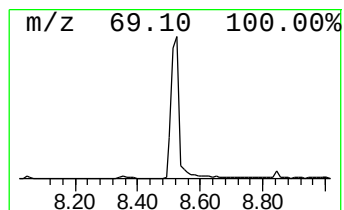
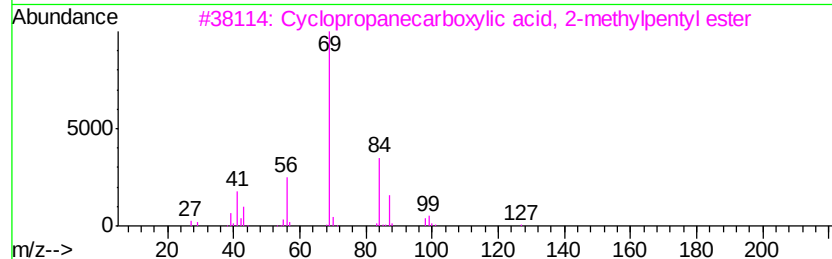
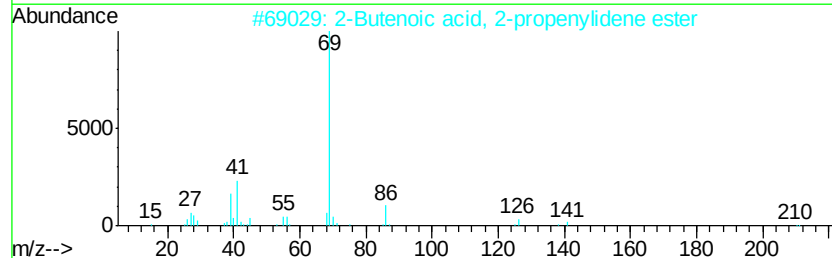
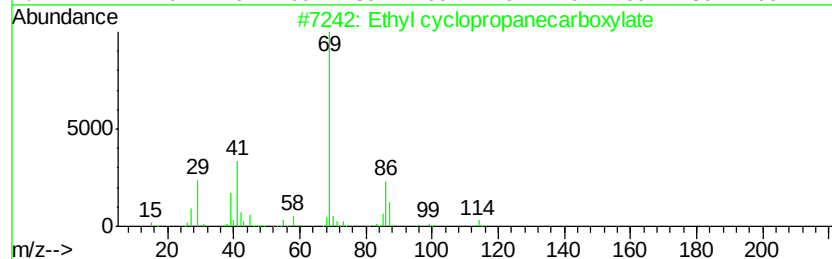
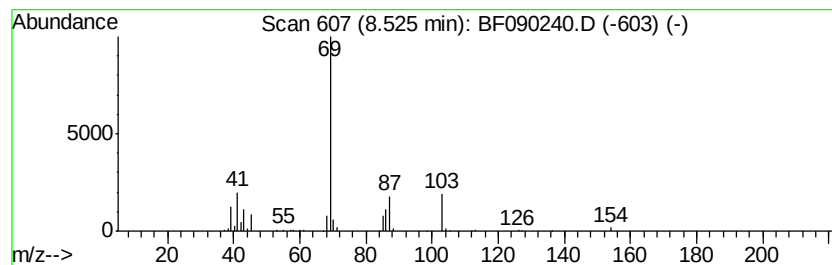
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Peak Number 6 unknown8.52 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	7.35 ng	411135	Napthalene-d8	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
2		2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
3		Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	33
4		Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9
5		2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	9



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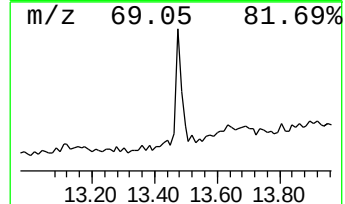
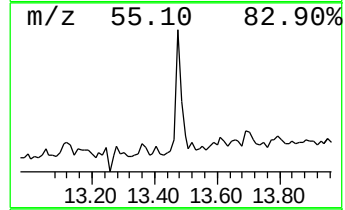
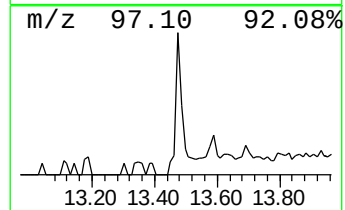
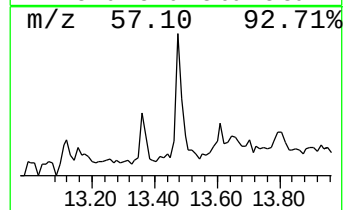
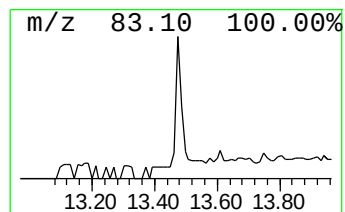
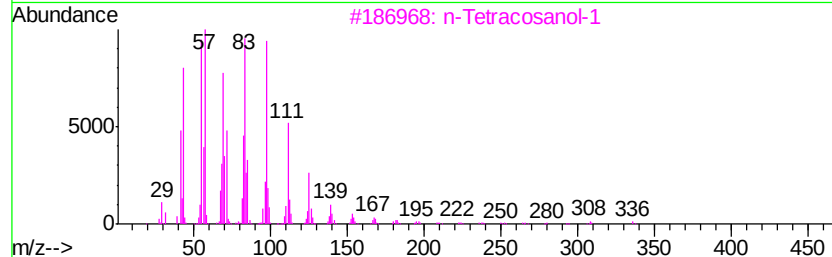
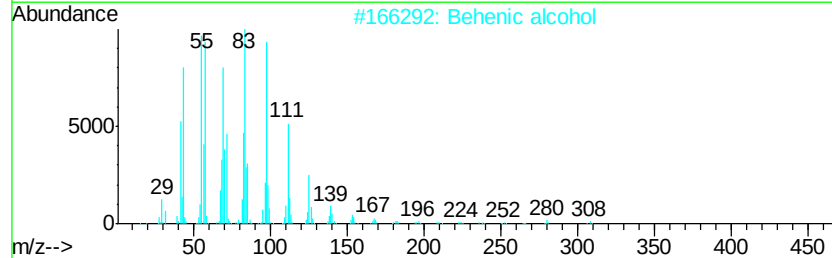
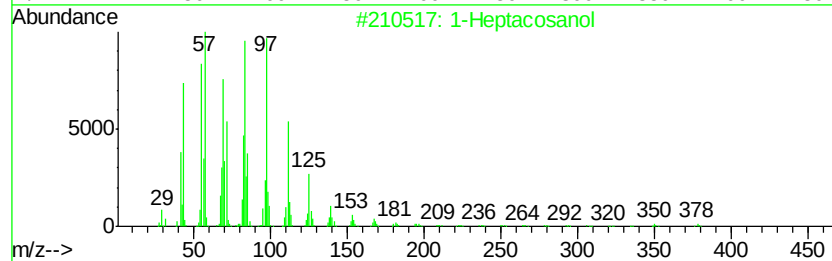
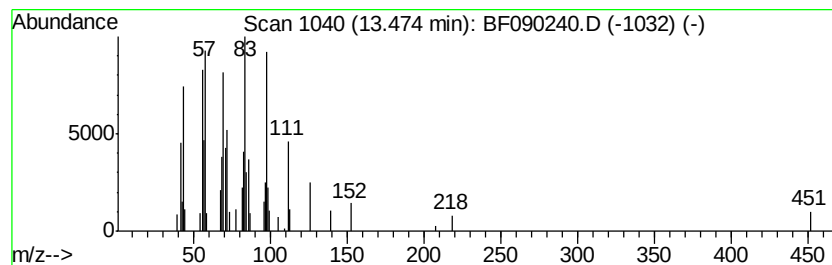
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Peak Number 7 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.03 ng	83839	Chrysene-d12	13.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	95
2	Behenic alcohol		326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	95
4	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	94
5	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94



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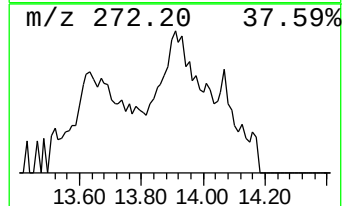
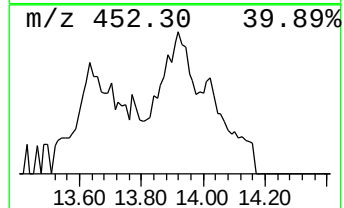
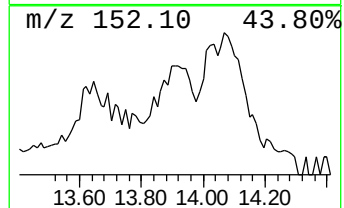
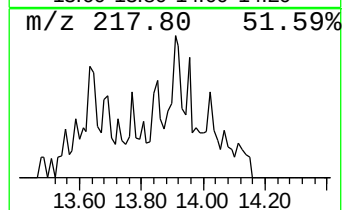
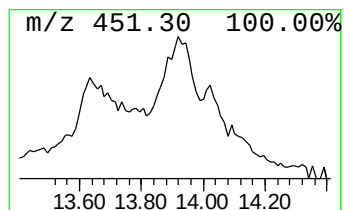
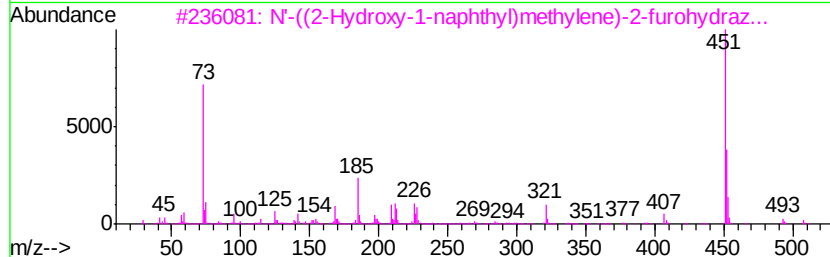
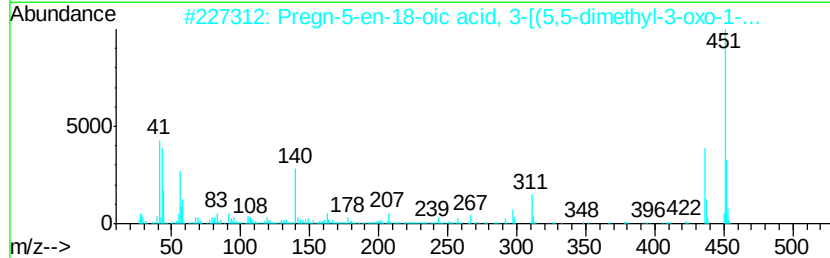
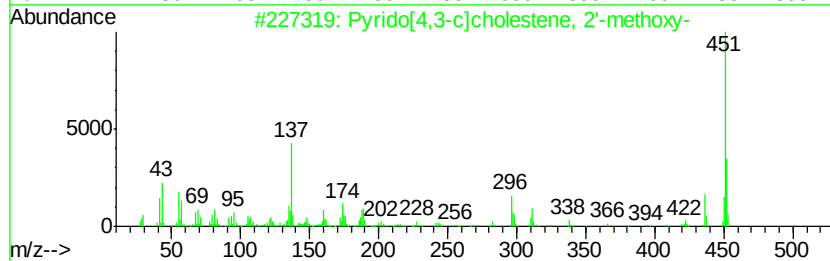
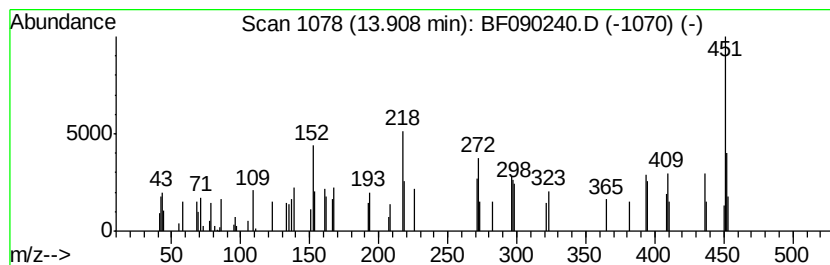
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Peak Number 8 unknown13.91 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.91	3.11 ng	128127	Chrysene-d12	13.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[4,3-c]cholestene, 2'-meth...	451	C31H49NO	1000210-91-7	38
2	Pregn-5-en-18-oic acid, 3-[(5,5-...	451	C29H41NO3	055401-43-9	25
3	N'-((2-Hydroxy-1-naphthyl)methyl...	508	C28H40N2O3Si2	1000331-88-6	25
4	Urs-12-ene	410	C30H50	000464-97-1	18
5	Cholest-3-eno[3,4-b]pyridine, 2'...	451	C31H49NO	1000210-91-6	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.55	4.5	ng	185574	1	6.48	833589	20.0
unknown6.24	6.24	48.9	ng	2038510	1	6.48	833589	20.0
unknown8.52	8.52	7.3	ng	411135	2	7.77	1119080	20.0
1-Heptacosanol	13.47	2.0	ng	83839	5	13.59	824878	20.0
unknown13.91	13.91	3.1	ng	128127	5	13.59	824878	20.0