

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051515\
 Data File : BF079283.D
 Acq On : 15 May 2015 21:35
 Operator : TP/IZ
 Sample : G2216-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-42

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-BF043015.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	1.461	21	24	36	rVB	221185	522103	10.97%	2.698%
2	1.621	36	38	41	rVV	488725	676244	14.21%	3.495%
3	1.667	41	42	51	rVV	177767	379380	7.97%	1.961%
4	1.792	51	53	97	rVB	2189534	4760164	100.00%	24.603%
5	4.947	327	329	335	rBV	69475	84191	1.77%	0.435%
6	5.461	372	374	377	rBV	539713	619055	13.00%	3.200%
7	6.742	483	486	489	rBV	449191	401947	8.44%	2.077%
8	6.890	496	499	501	rBV	1190113	1294819	27.20%	6.692%
9	7.176	521	524	526	rBV	392860	348996	7.33%	1.804%
10	7.359	538	540	543	rBV	1223883	1207960	25.38%	6.243%
11	7.873	582	585	587	rBV	930643	980160	20.59%	5.066%
12	8.753	659	662	664	rBV	528148	480688	10.10%	2.484%
13	10.102	777	780	782	rBV	2232635	2043093	42.92%	10.560%
14	10.925	850	852	855	rVB	578200	532822	11.19%	2.754%
15	11.256	879	881	884	rBV	43063	52284	1.10%	0.270%
16	11.908	935	938	940	rBV	1029287	1297933	27.27%	6.708%
17	12.765	1010	1013	1015	rBV	580054	554932	11.66%	2.868%
18	14.354	1149	1152	1155	rVB	56629	89263	1.88%	0.461%
19	14.765	1185	1188	1190	rBV	1341590	1869124	39.27%	9.661%
20	16.045	1298	1300	1303	rBV	497179	540574	11.36%	2.794%
21	17.223	1401	1403	1406	rBV	87734	100401	2.11%	0.519%
22	17.794	1451	1453	1456	rBV	423993	511847	10.75%	2.645%

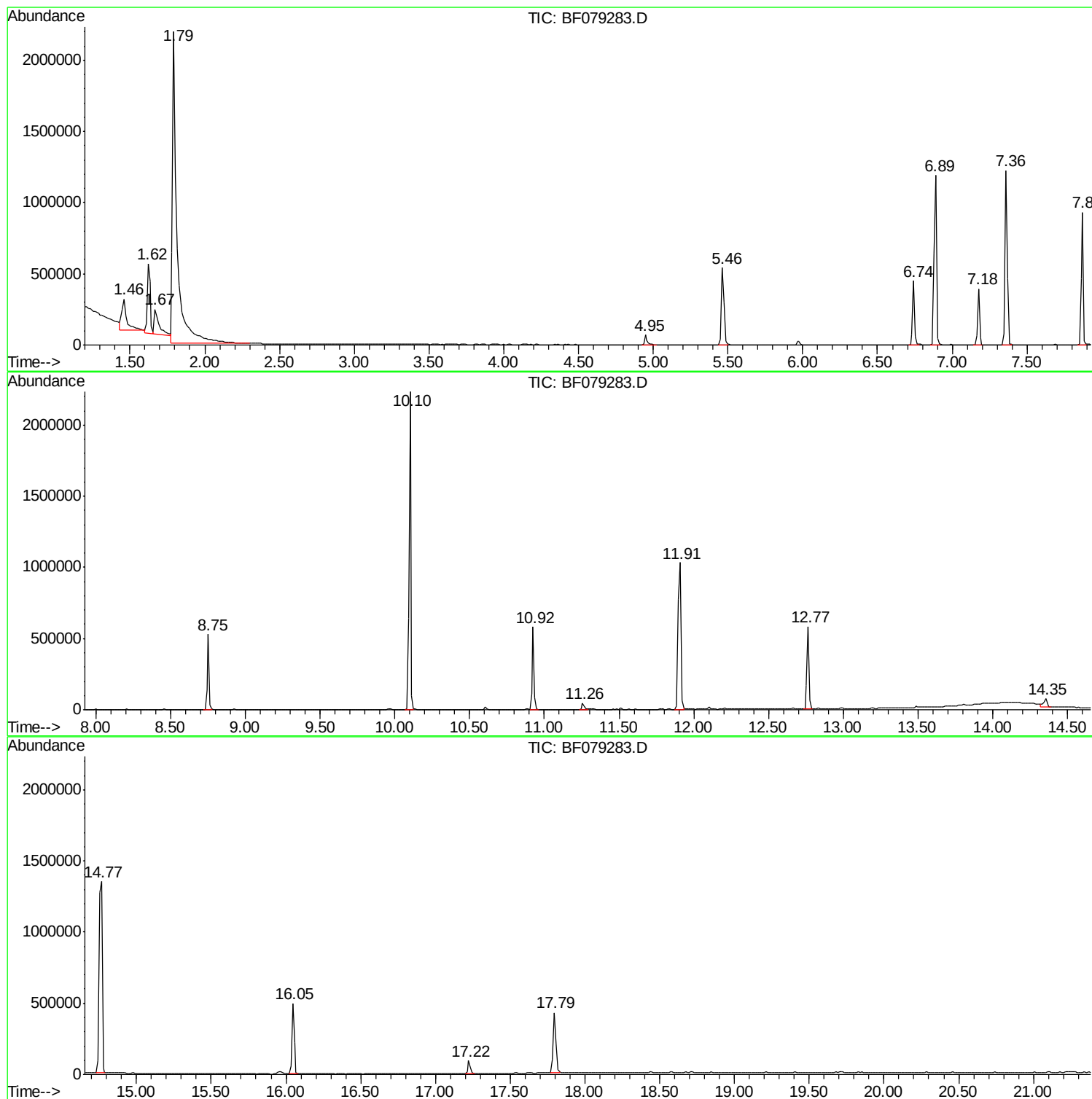
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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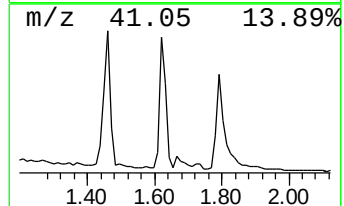
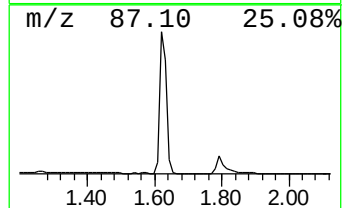
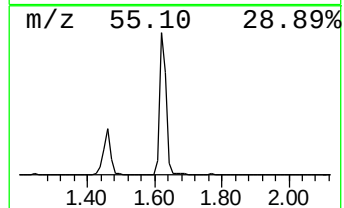
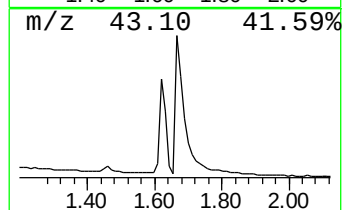
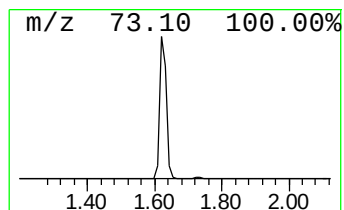
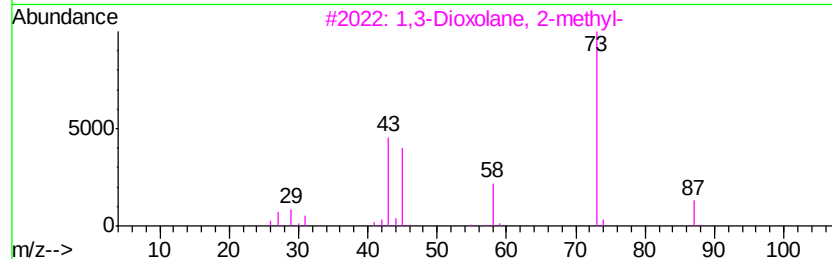
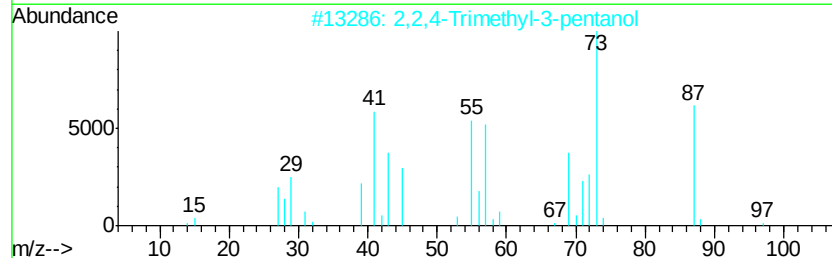
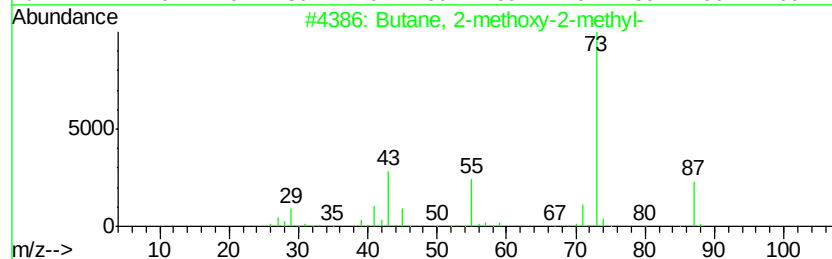
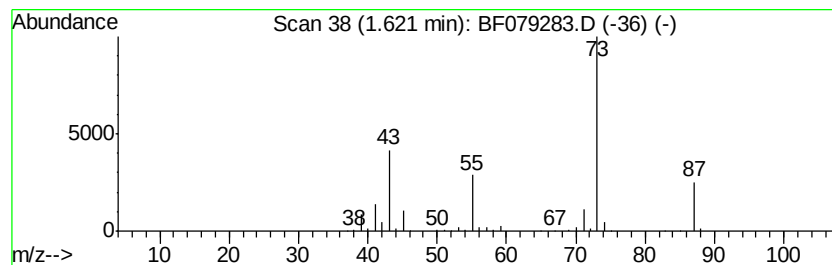
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	38.75 ng	676244	1,4-Dichlorobenzene-d4	7.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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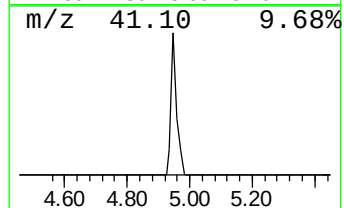
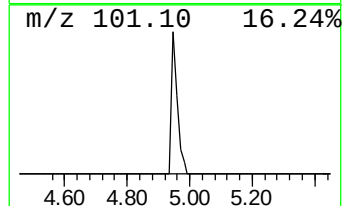
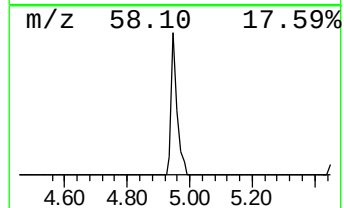
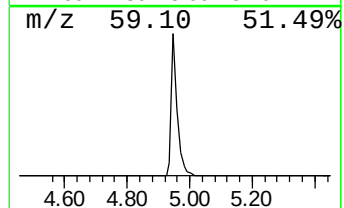
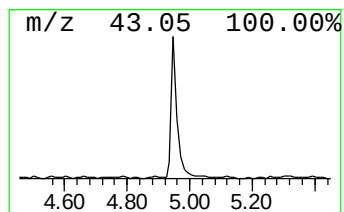
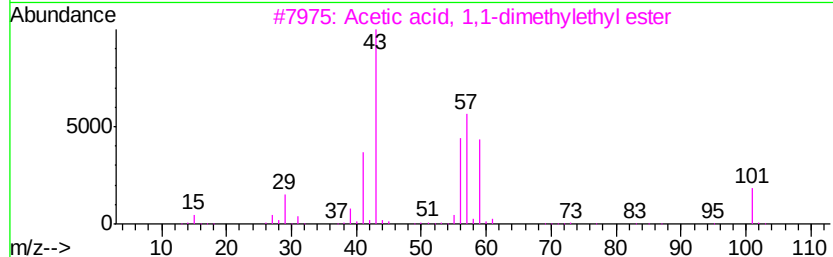
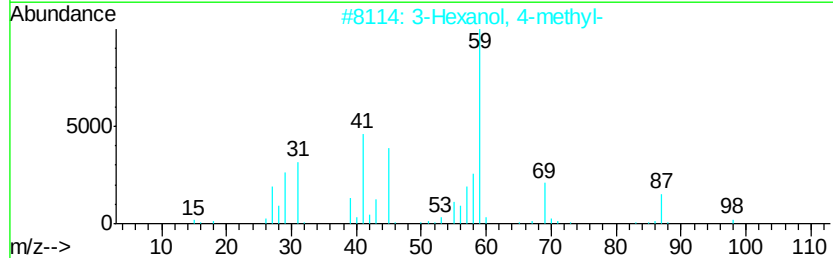
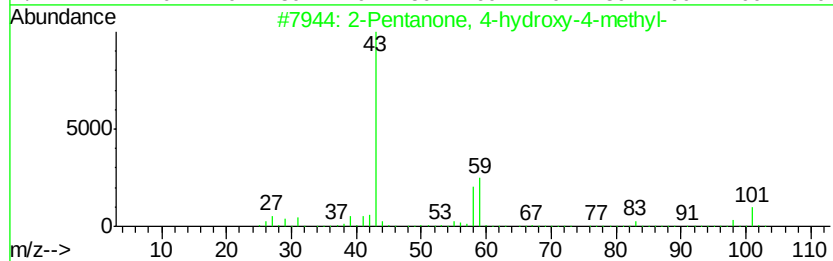
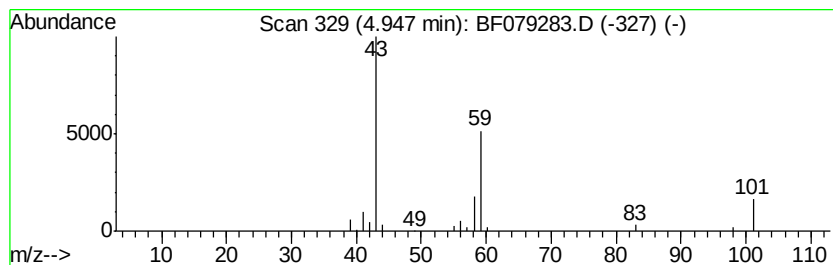
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	4.82 ng	84191	1,4-Dichlorobenzene-d4	7.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9		



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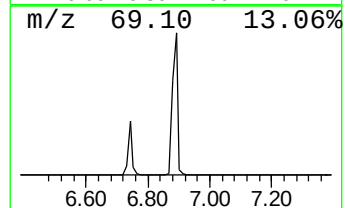
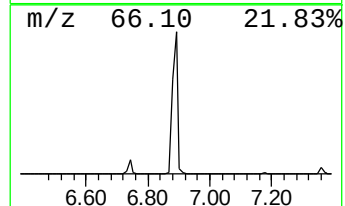
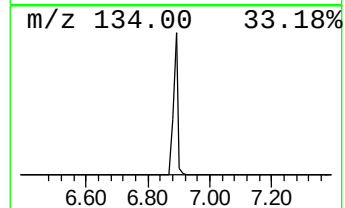
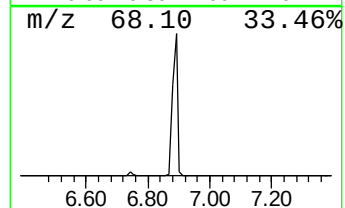
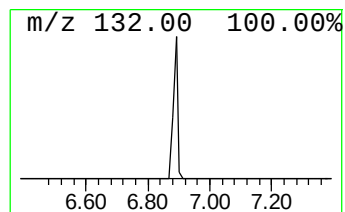
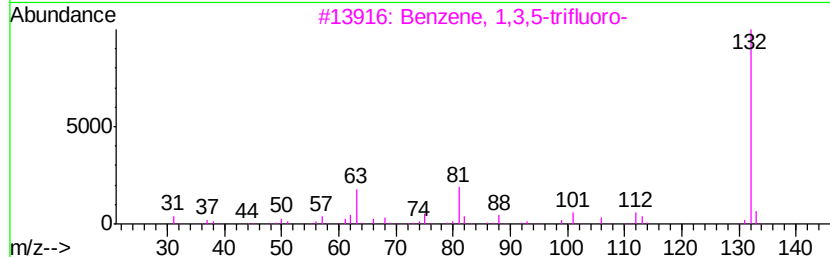
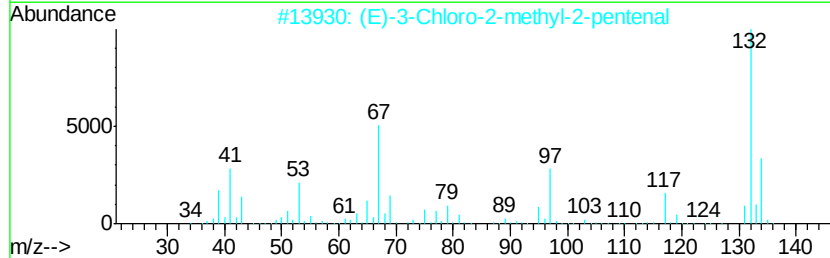
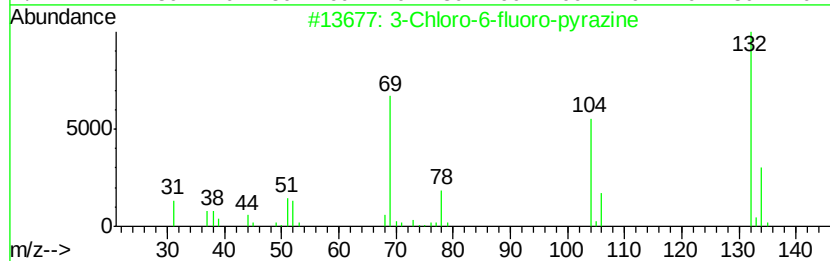
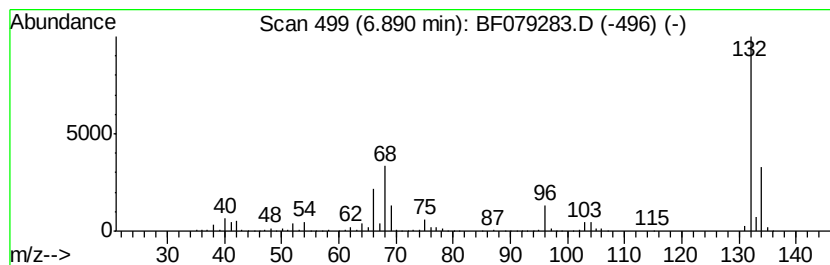
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Peak Number 6 unknown6.89 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	74.20 ng	1294820	1,4-Dichlorobenzene-d4	7.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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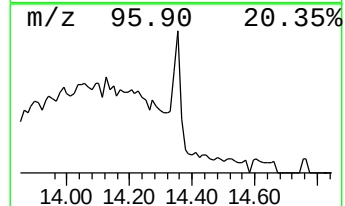
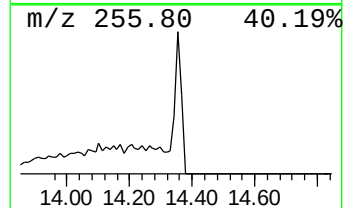
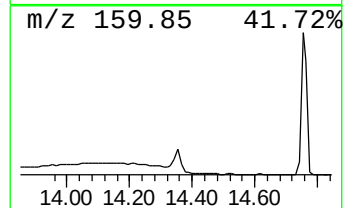
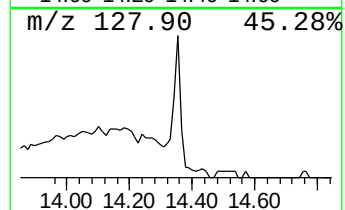
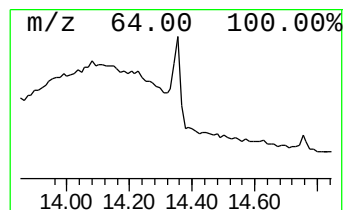
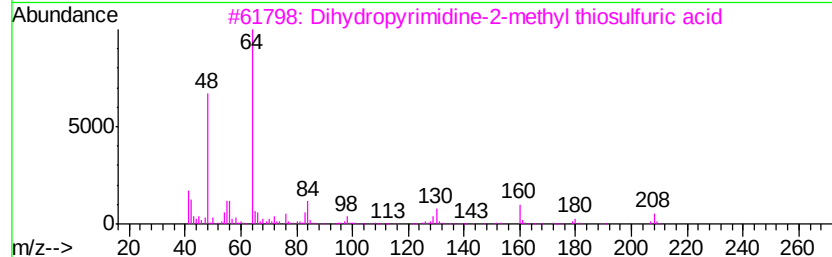
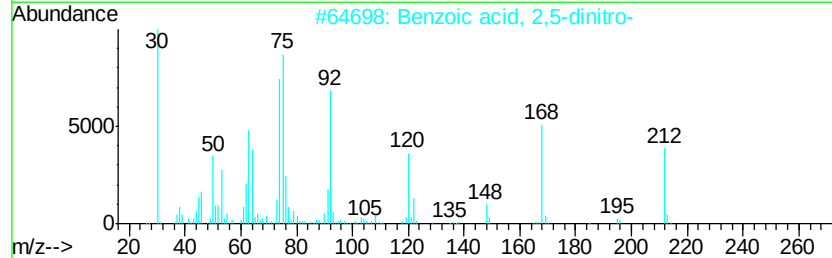
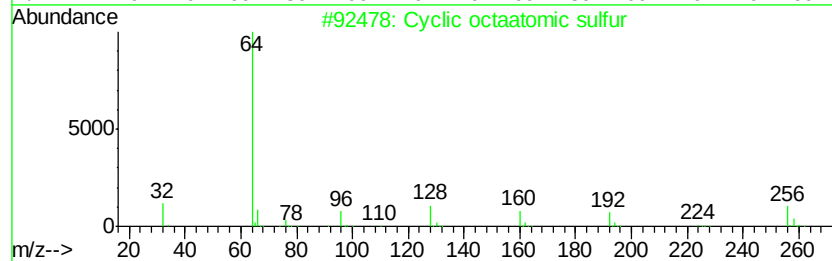
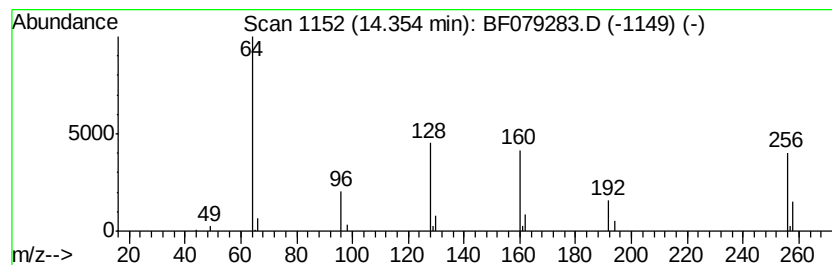
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Peak Number 8 Cyclic octaatomic sulfur Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.22 ng	89263	Phenanthrene-d10	12.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclic octaatomic sulfur	256	S8	010544-50-0	90
2		Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	50
3		Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	33
4		2-Norbornanone, 1-(epithioethyl)...	228	C11H16O3S	001782-93-0	9
5		Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2O2S	1000269-94-4	9



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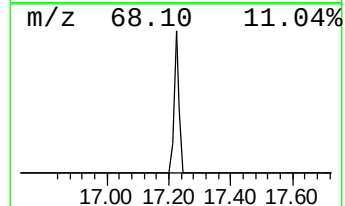
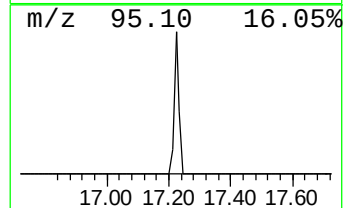
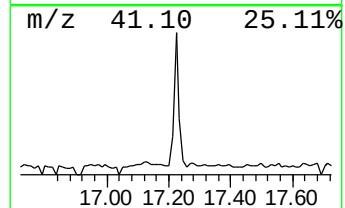
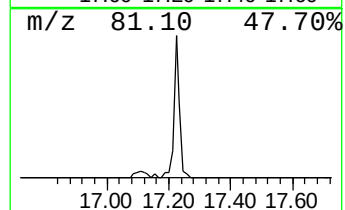
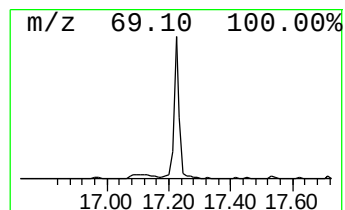
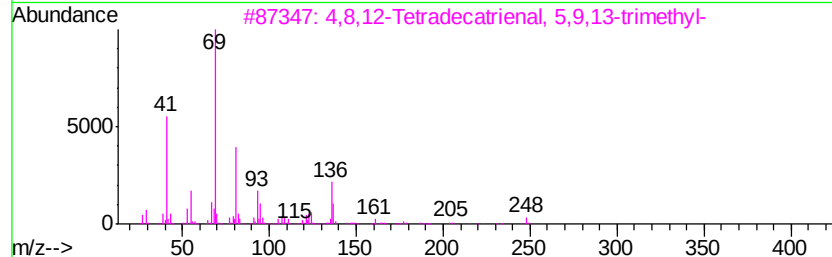
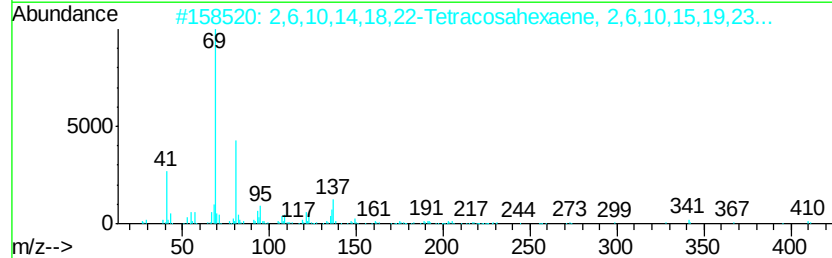
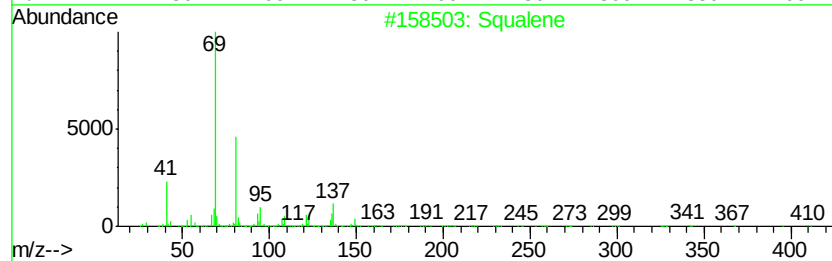
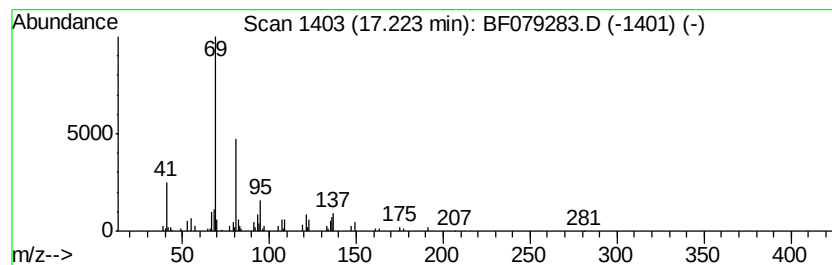
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Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	3.92 ng	100401	Perylene-d12	17.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53
5		Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.62	38.8	ng	676244	1	7.18	348996	20.0
2-Pentanone, 4-hy...	4.95	4.8	ng	84191	1	7.18	348996	20.0
unknown6.89	6.89	74.2	ng	1294820	1	7.18	348996	20.0
Cyclic octaatomic...	14.35	3.2	ng	89263	4	12.77	554932	20.0
Squalene	17.22	3.9	ng	100401	6	17.79	511847	20.0