

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
 Data File : BF117867.D
 Acq On : 19 Nov 2019 18:47
 Operator : JU
 Sample : K5865-18
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2-(6-8)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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	2.199	14	19	26	rVB	643514	853805	20.23%	2.287%
2	5.128	512	517	527	rVB	481159	563318	13.35%	1.509%
3	5.528	580	585	588	rBV	3216329	3004843	71.19%	8.051%
4	6.534	751	756	769	rBV	3741823	3641436	86.28%	9.756%
5	6.681	777	781	784	rBV	4014841	3602317	85.35%	9.651%
6	6.916	817	821	824	rBV	1470176	1177602	27.90%	3.155%
7	7.069	843	847	851	rBV	3238705	2842721	67.35%	7.616%
8	7.475	911	916	919	rBV	2573846	2216158	52.51%	5.937%
9	8.198	1035	1039	1043	rBV	1729186	1542851	36.55%	4.134%
10	9.281	1218	1223	1226	rBV	5170231	4220643	100.00%	11.308%
11	9.675	1286	1290	1293	rBV	437159	385371	9.13%	1.032%
12	9.963	1335	1339	1343	rBV	2250672	1815931	43.02%	4.865%
13	10.751	1469	1473	1477	rBV	2647584	2258948	53.52%	6.052%
14	11.457	1589	1593	1596	rBV	2095455	1760585	41.71%	4.717%
15	11.522	1598	1604	1608	rVB4	61447	59578	1.41%	0.160%
16	13.045	1859	1863	1866	rBV	4426522	3751000	88.87%	10.050%
17	13.969	2013	2020	2033	rBV3	74894	241446	5.72%	0.647%
18	14.104	2039	2043	2047	rVB	1539463	1322821	31.34%	3.544%
19	14.568	2119	2122	2125	rBV	64311	66434	1.57%	0.178%
20	14.886	2173	2176	2180	rVB	94451	98937	2.34%	0.265%
21	14.968	2186	2190	2194	rBV	97972	97220	2.30%	0.260%
22	15.245	2232	2237	2243	rVB	99561	123709	2.93%	0.331%
23	15.610	2293	2299	2303	rBV	1011484	1296312	30.71%	3.473%
24	15.645	2303	2305	2316	rVB2	101592	120057	2.84%	0.322%
25	16.104	2378	2383	2388	rVB2	73851	112650	2.67%	0.302%
26	16.639	2469	2474	2480	rVB2	47465	88664	2.10%	0.238%
27	17.268	2575	2581	2588	rBV5	26729	59458	1.41%	0.159%

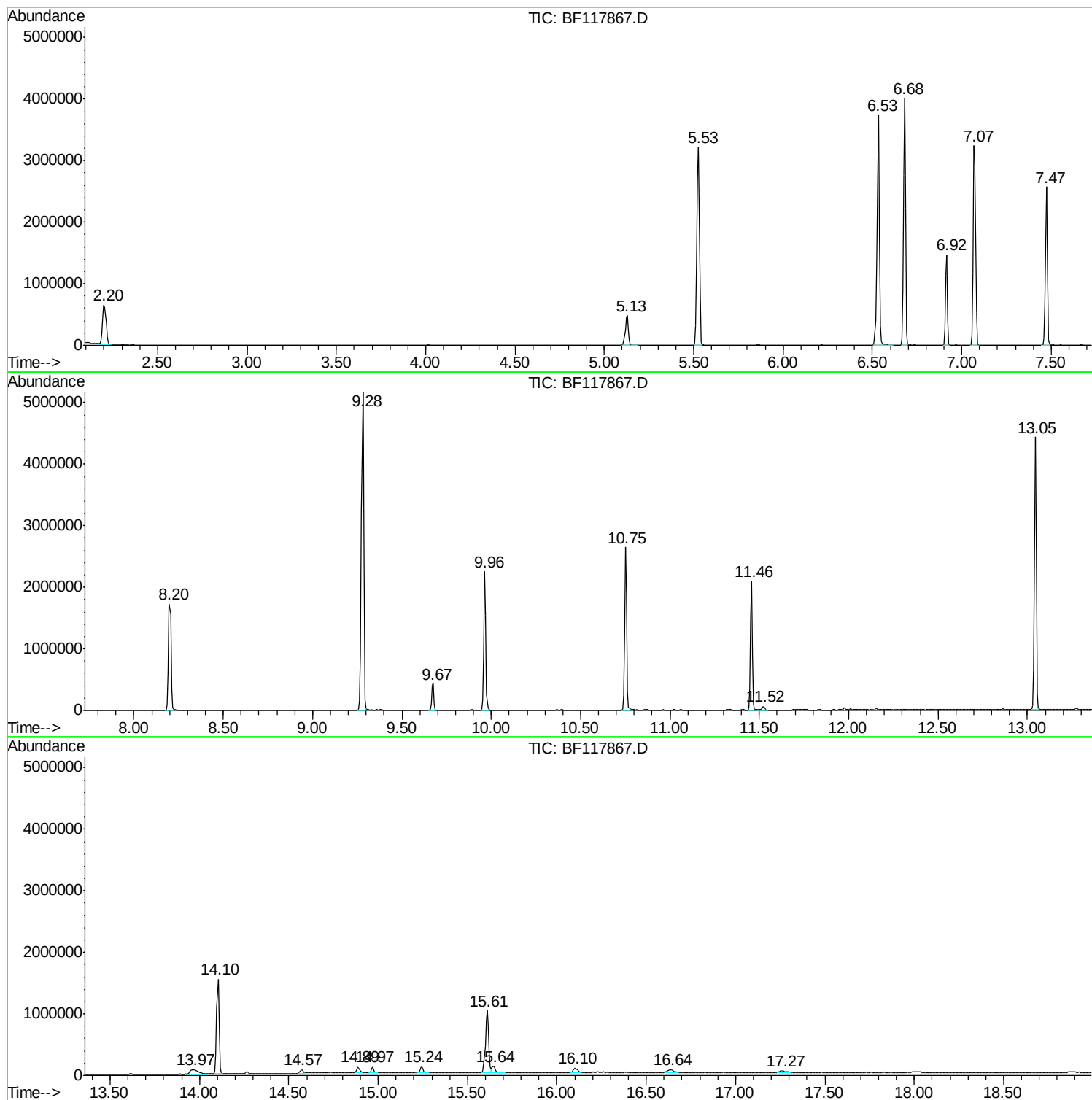
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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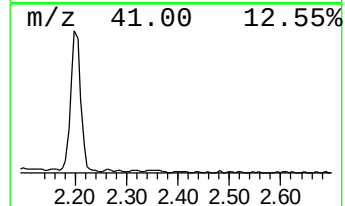
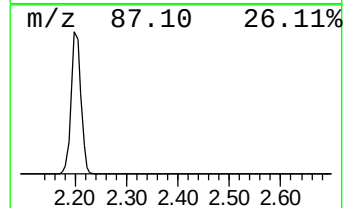
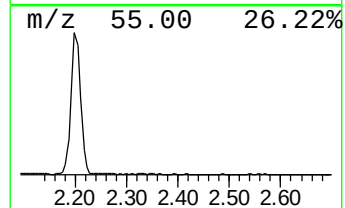
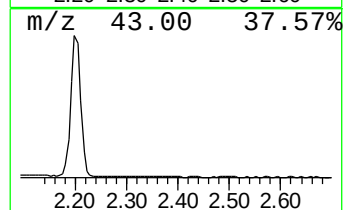
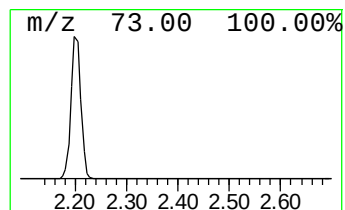
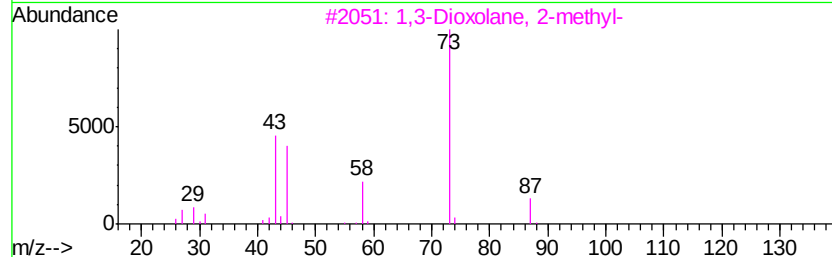
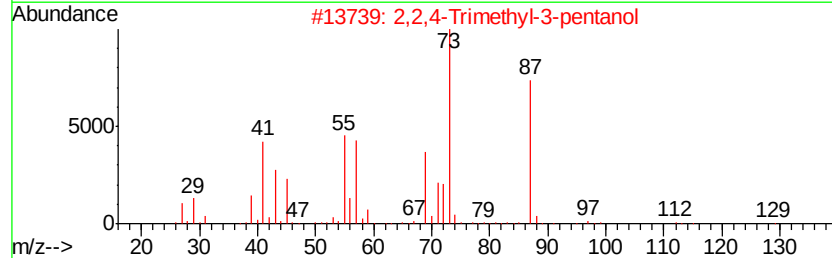
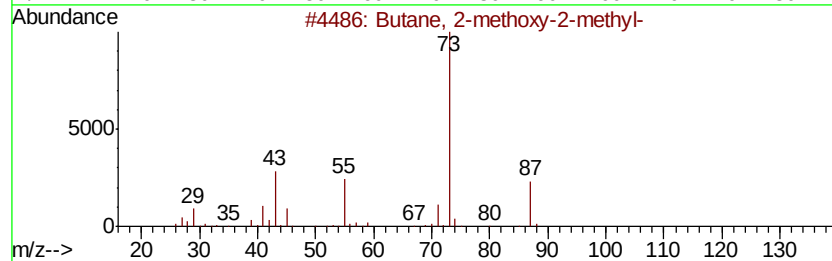
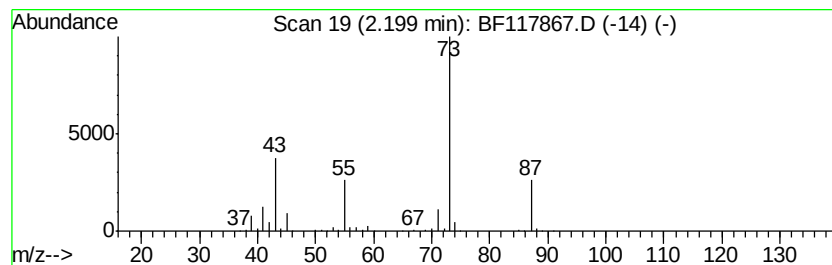
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	14.50 ng	853805	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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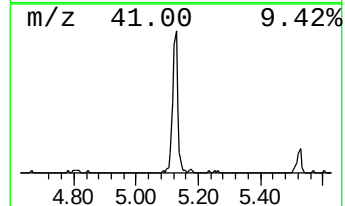
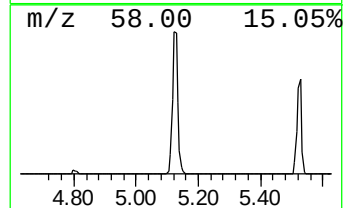
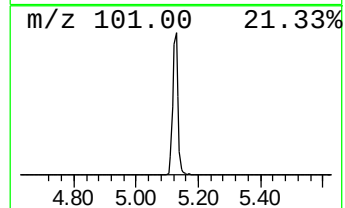
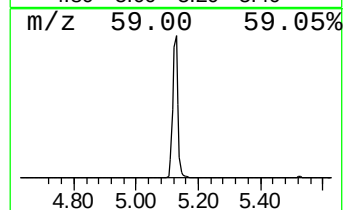
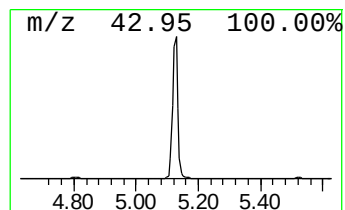
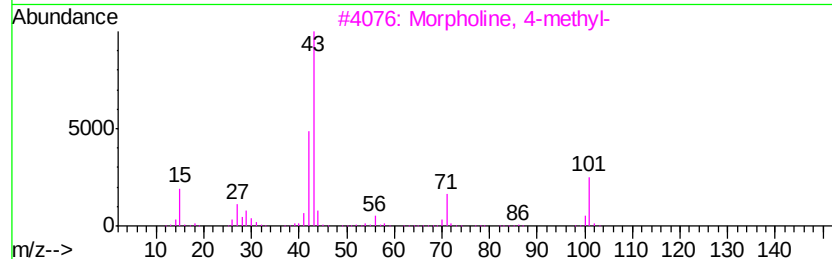
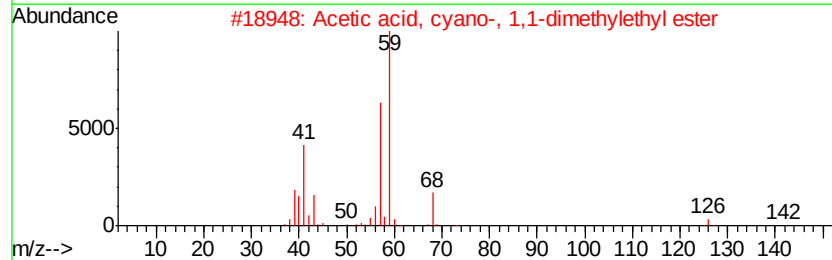
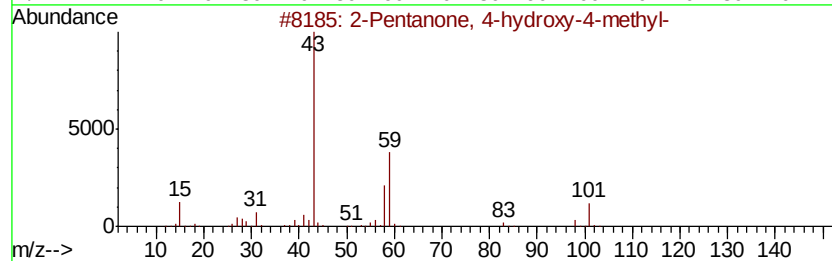
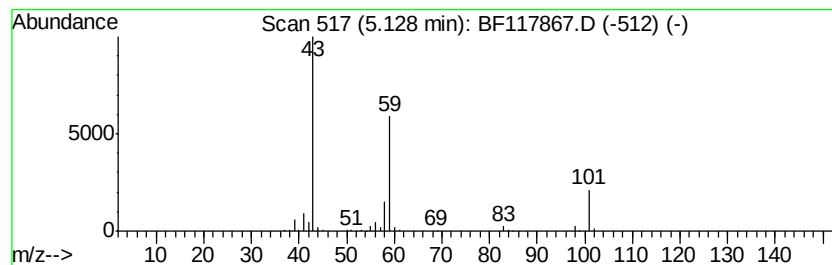
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	9.57 ng	563318	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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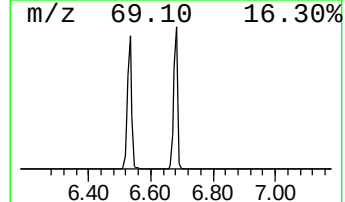
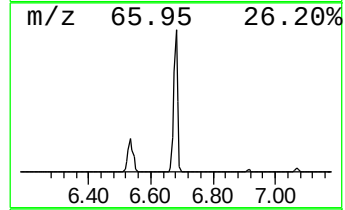
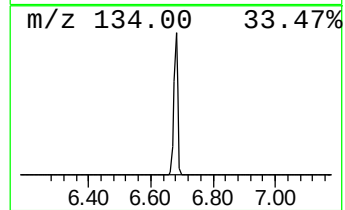
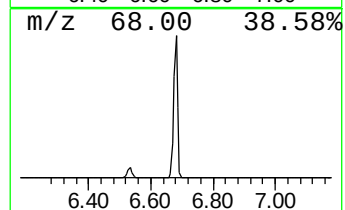
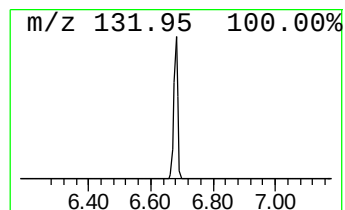
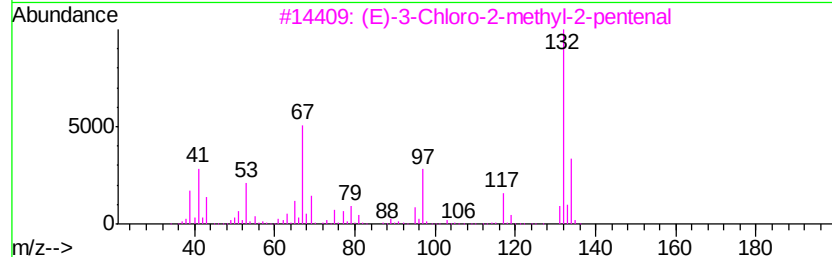
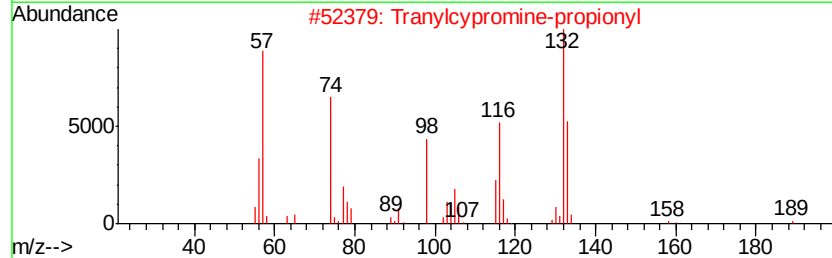
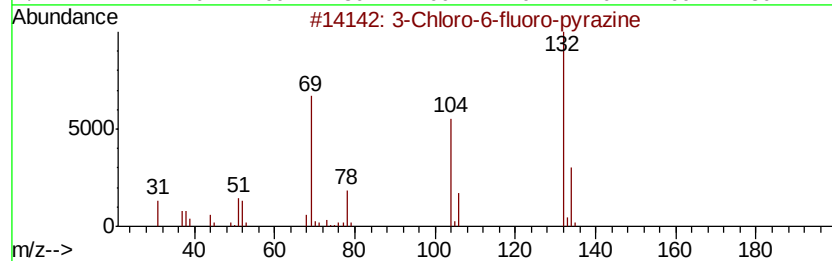
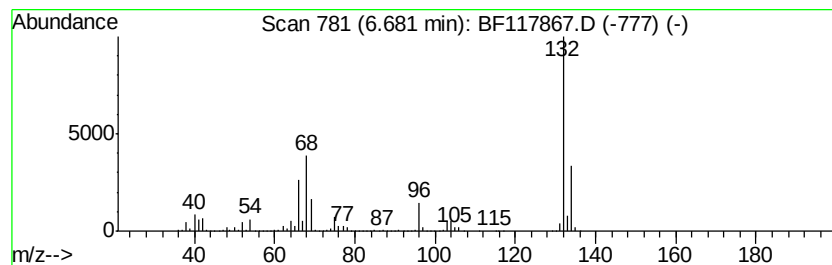
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Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	61.18 ng	3602320	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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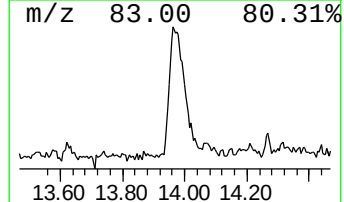
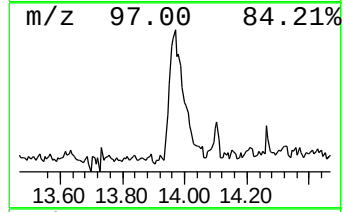
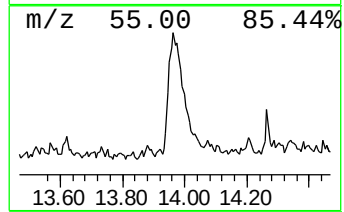
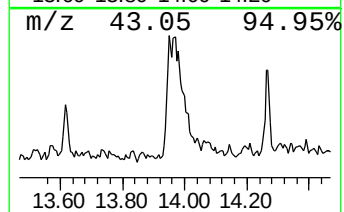
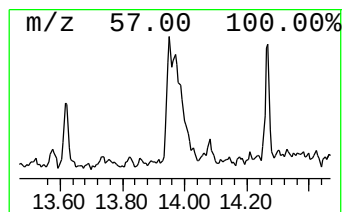
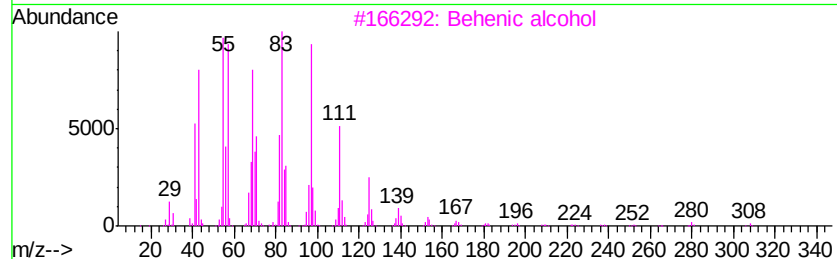
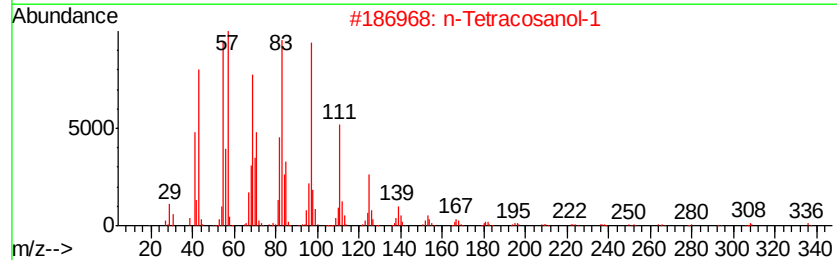
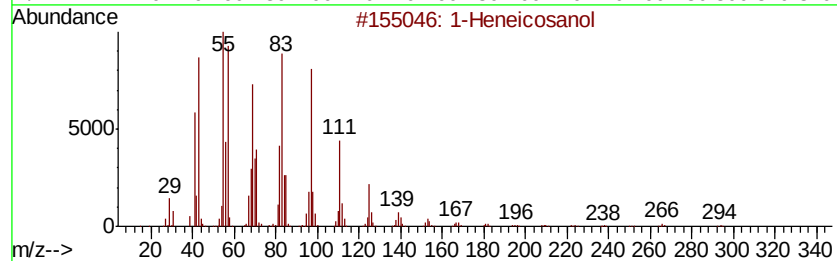
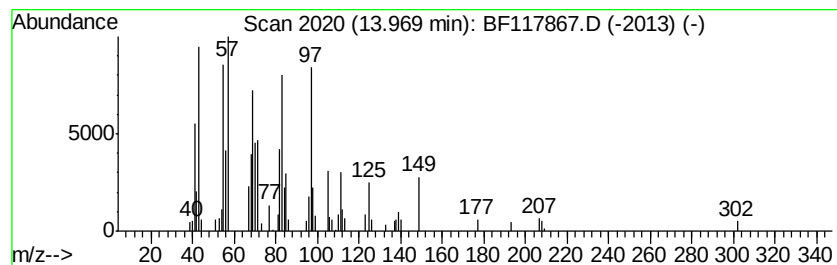
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.65 ng	241446	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	87
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3		Behenic alcohol	326	C22H46O	000661-19-8	87
4		Octacosanol	410	C28H58O	000557-61-9	87
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	14.5	ng	853805	1	6.92	1177600	20.0
2-Pentanone, 4-hy...	5.13	9.6	ng	563318	1	6.92	1177600	20.0
unknown6.68	6.68	61.2	ng	3602320	1	6.92	1177600	20.0
1-Heneicosanol	13.97	3.6	ng	241446	5	14.10	1322820	20.0