

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030619\
 Data File : BG039790.D
 Acq On : 6 Mar 2019 16:48
 Operator : JU/SJ
 Sample : K1704-12
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PST-028-SW003-022719

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_G\METHODS\8270-BG030419.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	3.208	15	20	29	rBV	73093	141681	4.14%	0.753%
2	3.284	29	33	42	rVB	39333	62689	1.83%	0.333%
3	5.699	437	444	458	rBV	870134	1383076	40.44%	7.354%
4	7.302	709	717	728	rBV	937307	1658486	48.50%	8.818%
5	7.684	773	782	792	rVV	853781	1466036	42.87%	7.795%
6	8.154	855	862	873	rVB	156247	269583	7.88%	1.433%
7	8.477	910	917	926	rBV	542042	943109	27.58%	5.015%
8	9.335	1055	1063	1072	rBV	514079	934704	27.33%	4.970%
9	10.974	1334	1342	1351	rBV	229838	414354	12.12%	2.203%
10	13.406	1744	1756	1763	rBV	1456225	2289825	66.96%	12.175%
11	14.222	1888	1895	1900	rBV	82333	117222	3.43%	0.623%
12	14.780	1982	1990	2001	rBV2	389607	647282	18.93%	3.442%
13	16.267	2232	2243	2253	rBV	1342647	1998927	58.45%	10.628%
14	17.524	2451	2457	2468	rVB2	536143	840796	24.59%	4.471%
15	18.375	2591	2602	2607	rBV4	45637	73648	2.15%	0.392%
16	20.120	2892	2899	2905	rBV	2593664	3419803	100.00%	18.183%
17	21.407	3113	3118	3127	rBV	57614	118083	3.45%	0.628%
18	21.812	3178	3187	3194	rBV	553304	927804	27.13%	4.933%
19	23.304	3432	3441	3448	rBV4	22885	47941	1.40%	0.255%
20	23.504	3469	3475	3481	rBV3	17372	34631	1.01%	0.184%
21	24.138	3577	3583	3589	rBV4	22149	48922	1.43%	0.260%
22	25.184	3747	3761	3773	rVB2	302683	926868	27.10%	4.928%
23	26.312	3945	3953	3958	rBV5	15169	41868	1.22%	0.223%

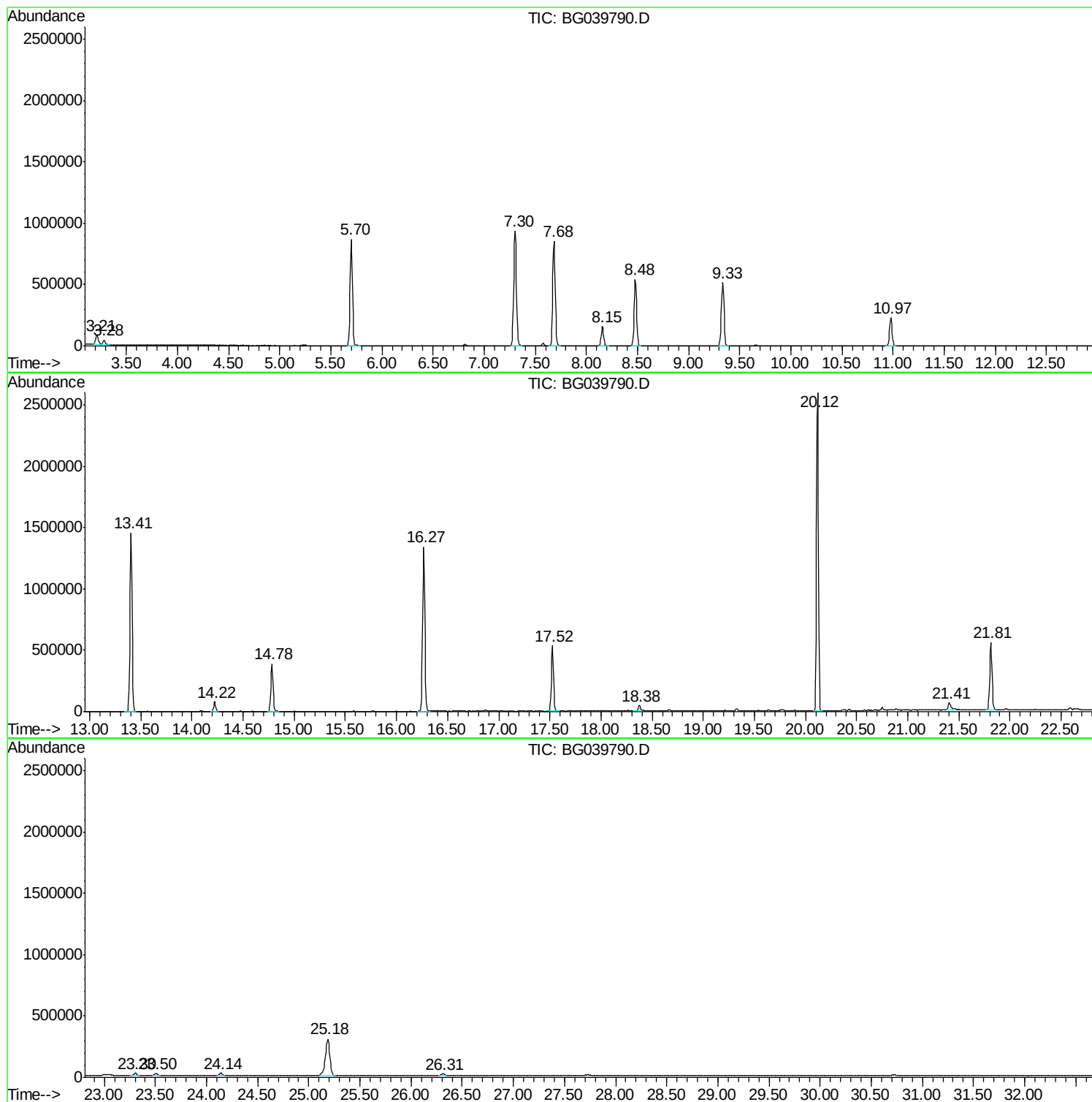
Sum of corrected areas: 18807338

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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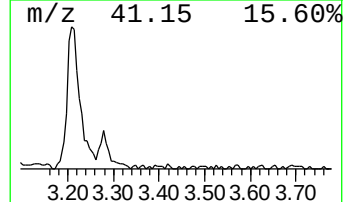
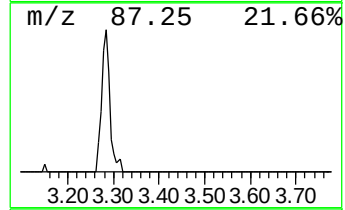
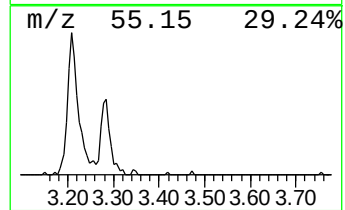
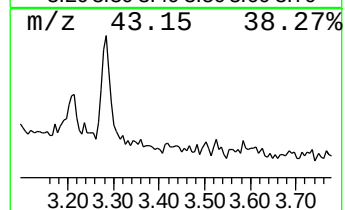
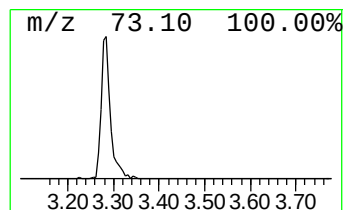
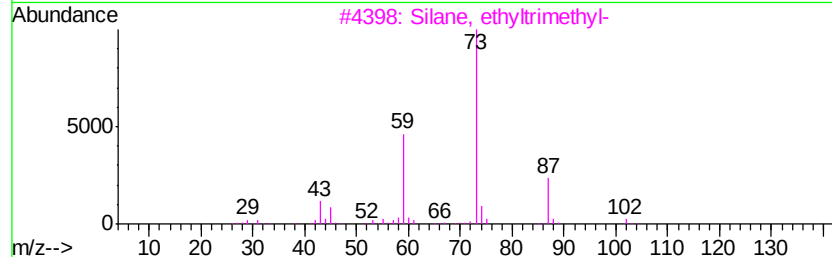
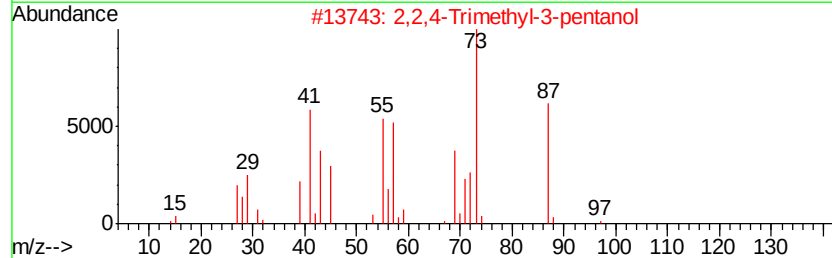
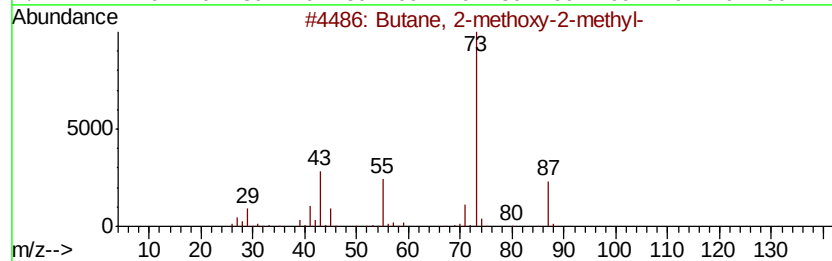
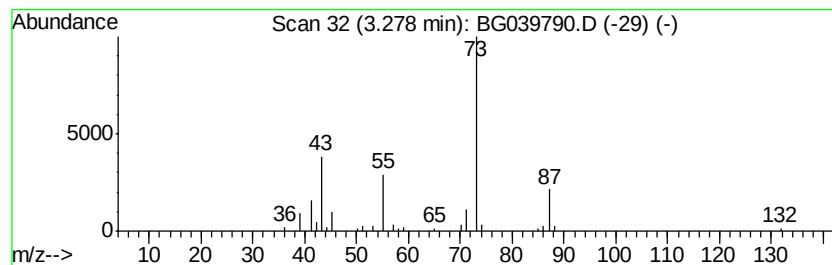
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	4.65 ng	62689	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
5			1,3-Dioxolane, 2-butyl-	130	C7H14O2	004360-76-3	17



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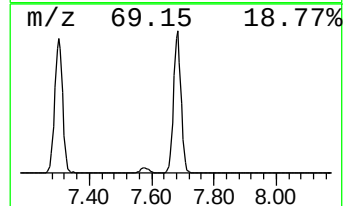
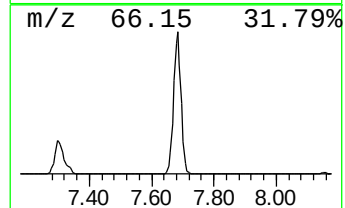
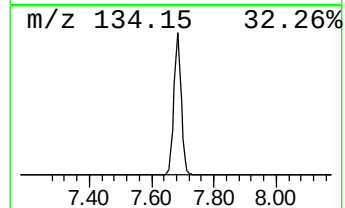
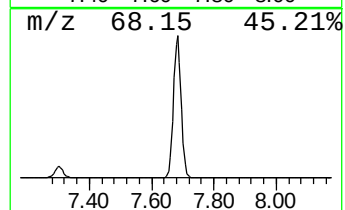
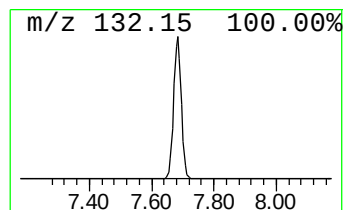
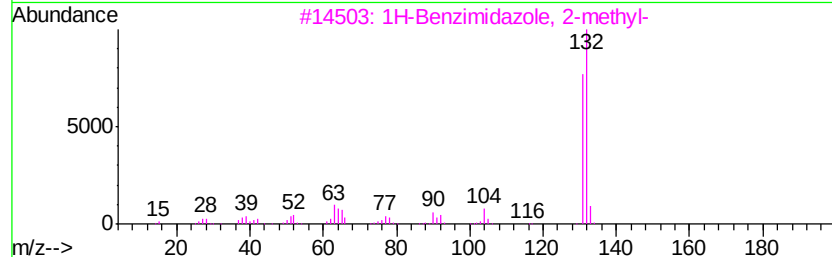
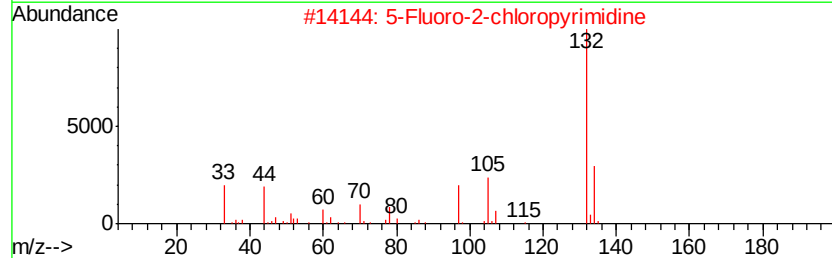
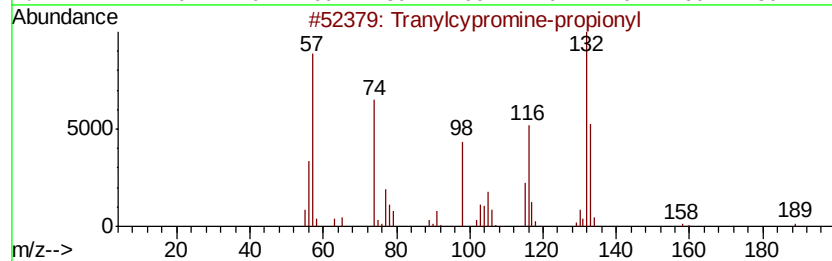
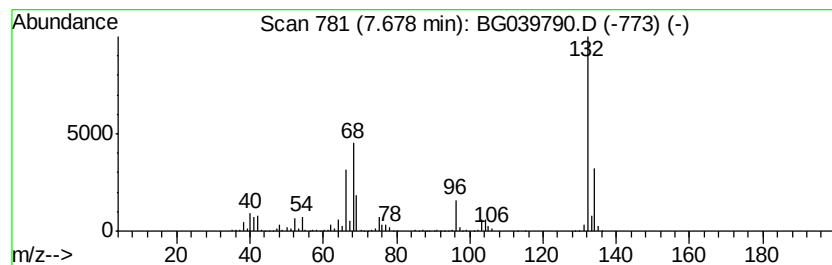
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Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	108.76 ng	1466040	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		N-(-3,4-Methylenedioxyphenyl)isopropylamine	267	C17H17NO2	1000378-96-6	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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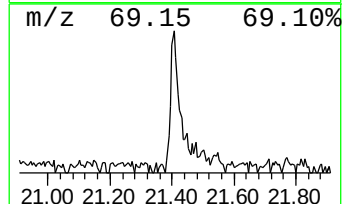
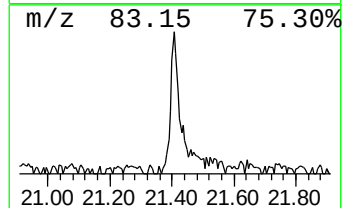
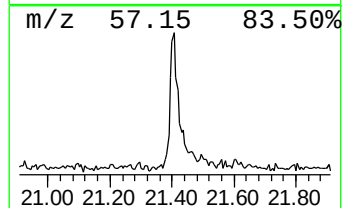
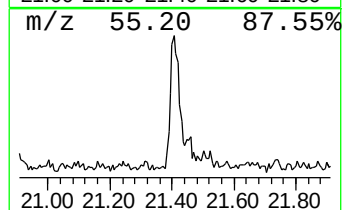
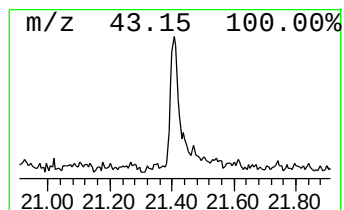
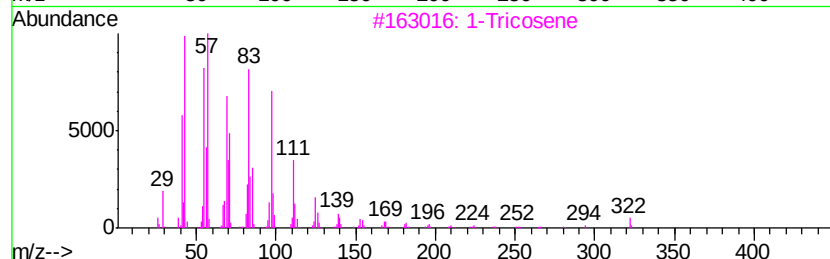
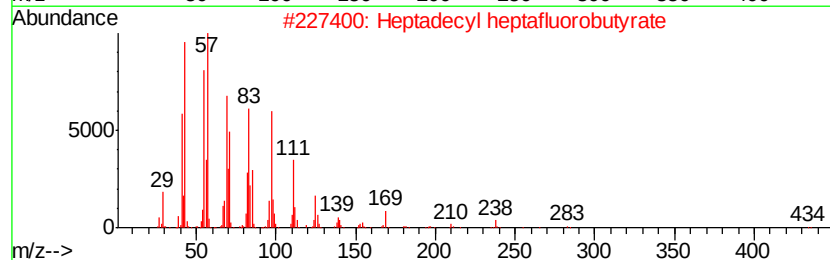
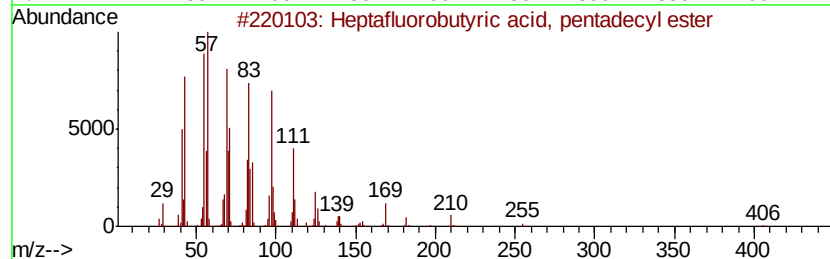
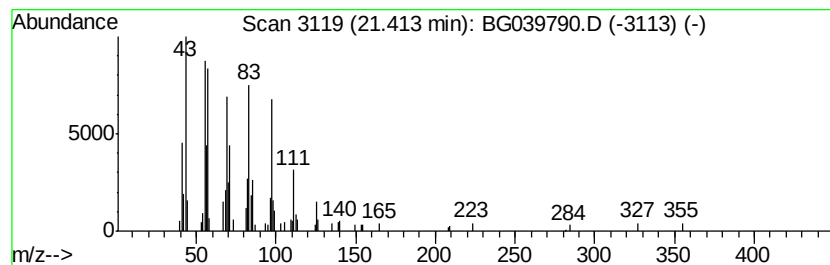
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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	2.55 ng	118083	Chrysene-d12	21.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		1-Tricosene	322	C23H46	018835-32-0	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.28	4.7	ng	62689	1	8.16	269583	20.0
unknown7.68	7.68	108.8	ng	1466040	1	8.16	269583	20.0
Heptafluorobutyri...	21.41	2.5	ng	118083	5	21.81	927804	20.0