

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
 Data File : BF097504.D
 Acq On : 9 Aug 2017 8:31
 Operator : SJ/JU
 Sample : PB101261BL
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB101261BL

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-BF072517.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	3.822	343	346	356	rBV2	33320	77767	2.94%	0.384%
2	4.545	464	469	487	rBV	518791	934045	35.32%	4.615%
3	5.010	545	548	573	rBV	2039438	2644570	100.00%	13.065%
4	6.081	726	730	743	rBV	2248884	2426958	91.77%	11.990%
5	6.181	743	747	764	rVB	2490072	2577516	97.46%	12.734%
6	6.404	782	785	797	rVB	620033	571932	21.63%	2.826%
7	6.563	808	812	828	rBV	1752139	1859295	70.31%	9.186%
8	6.981	879	883	912	rBV	1489919	1593402	60.25%	7.872%
9	7.686	1000	1003	1017	rBV	792205	745204	28.18%	3.682%
10	8.769	1182	1187	1190	rBV	2400668	2302384	87.06%	11.375%
11	9.433	1296	1300	1310	rBV	686519	640642	24.22%	3.165%
12	10.222	1430	1434	1456	rBV	1002409	999685	37.80%	4.939%
13	10.904	1547	1550	1560	rBV	544563	505440	19.11%	2.497%
14	12.333	1789	1793	1797	rBV	34539	27239	1.03%	0.135%
15	12.486	1815	1819	1823	rBV	1550051	1563930	59.14%	7.726%
16	13.527	1993	1996	2009	rVB	431458	449591	17.00%	2.221%
17	14.868	2220	2224	2234	rVB	262684	321629	12.16%	1.589%

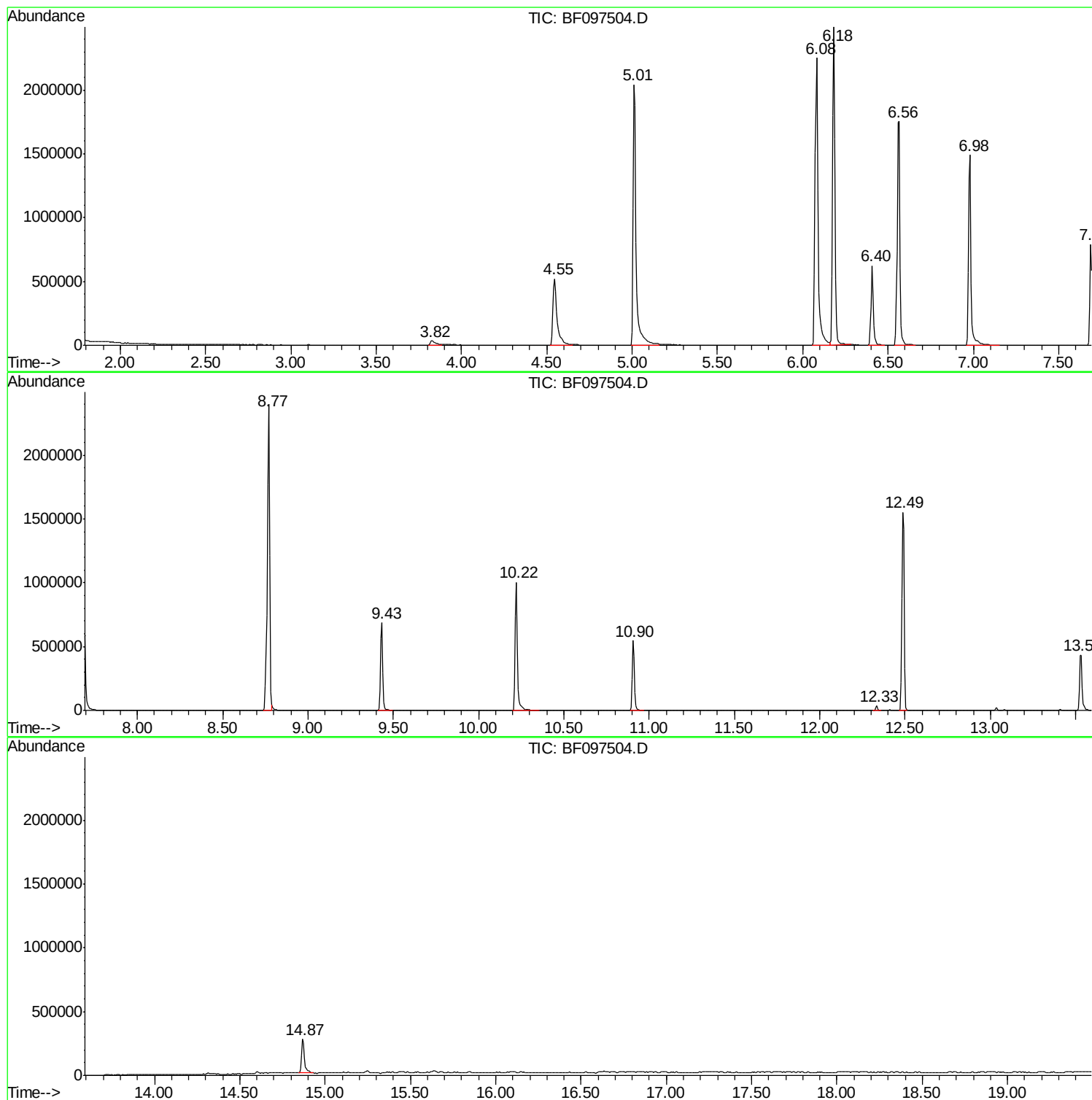
Sum of corrected areas: 20241229

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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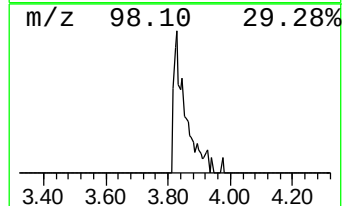
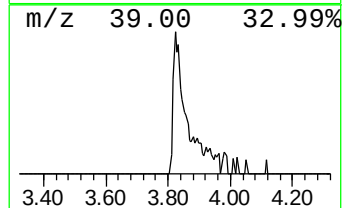
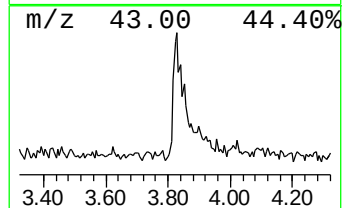
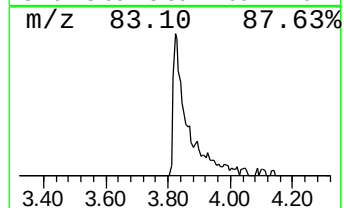
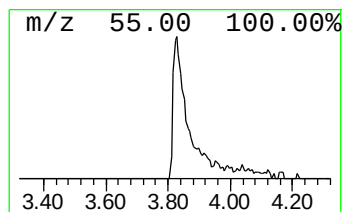
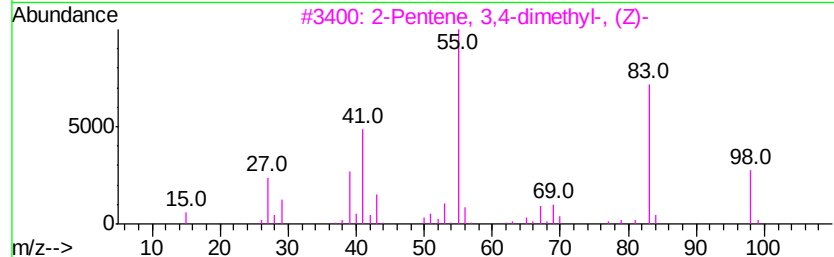
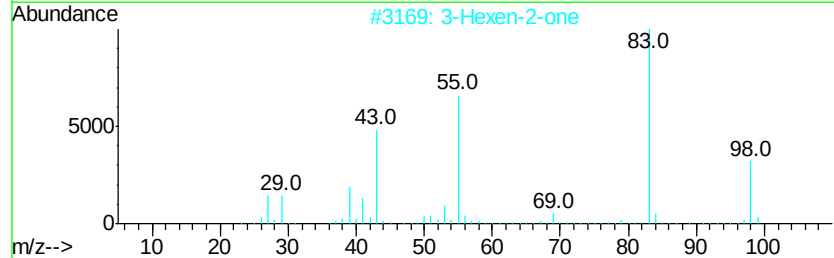
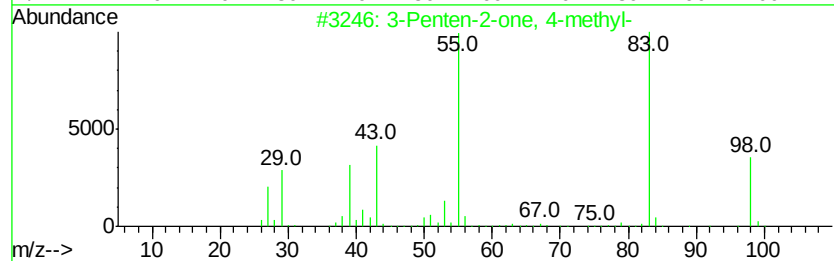
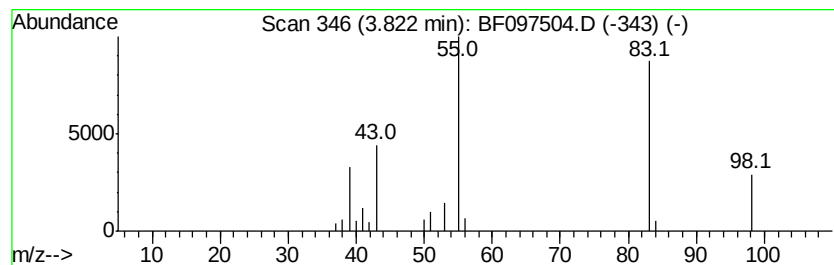
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.82	2.72 ng	77767	1,4-Dichlorobenzene-d4	6.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64



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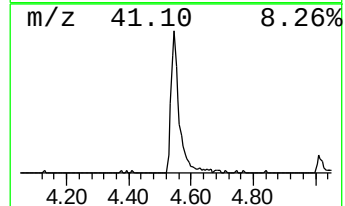
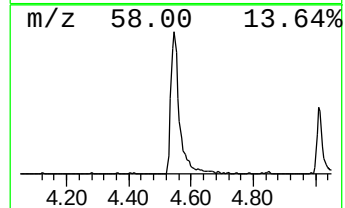
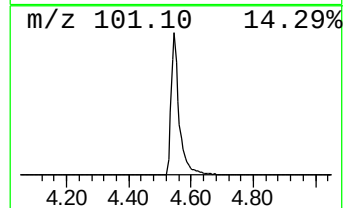
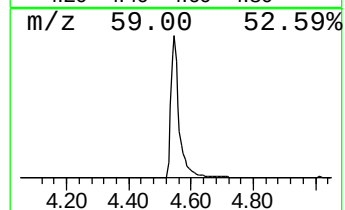
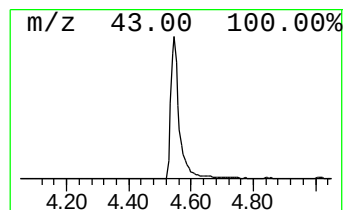
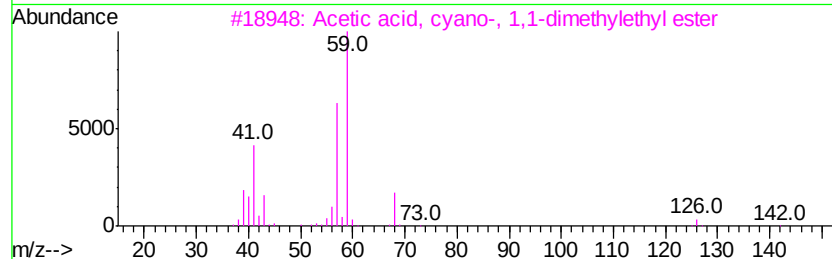
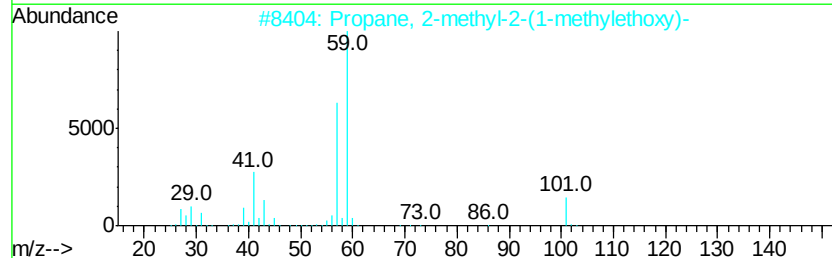
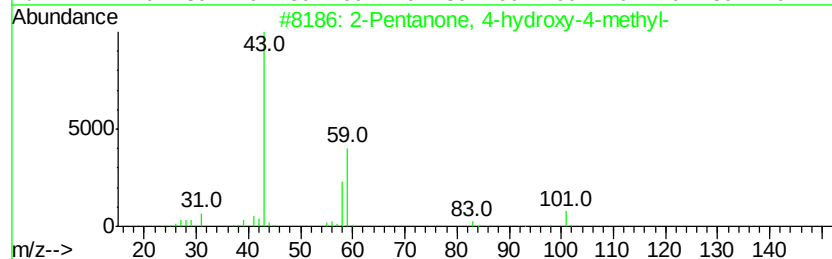
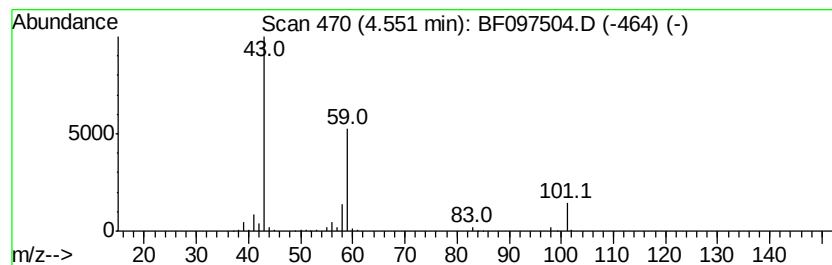
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	32.66 ng	934045	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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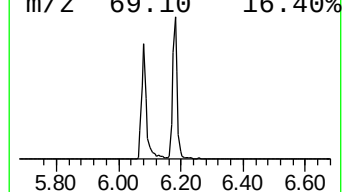
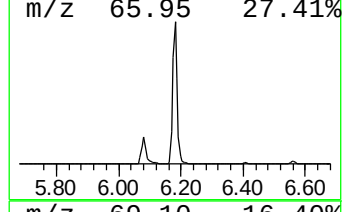
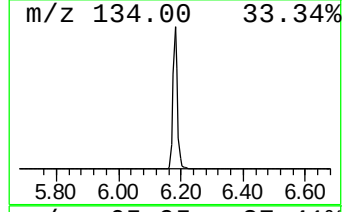
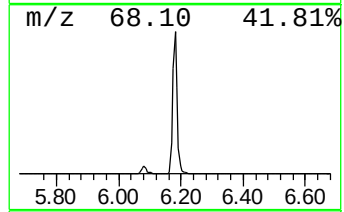
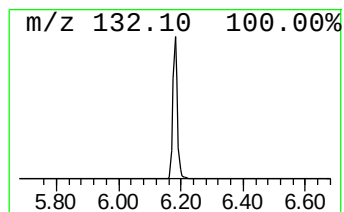
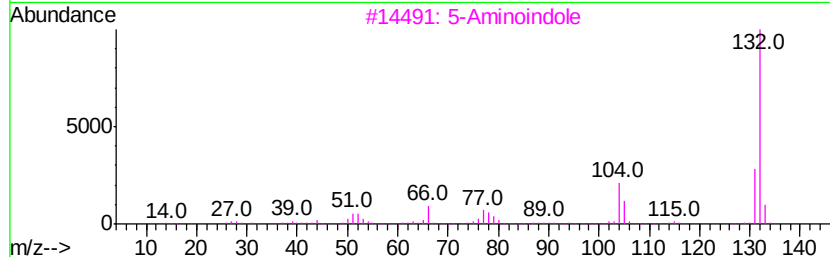
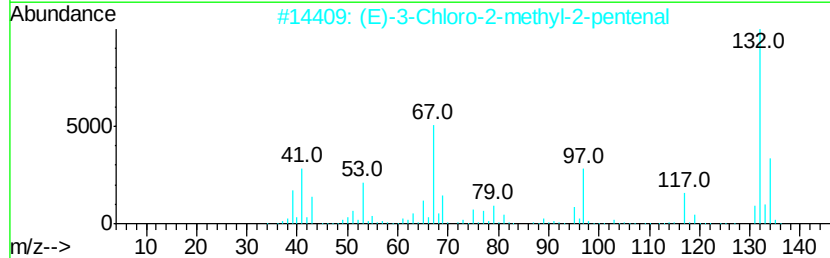
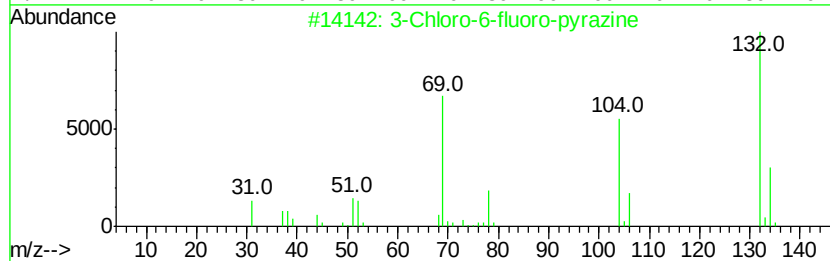
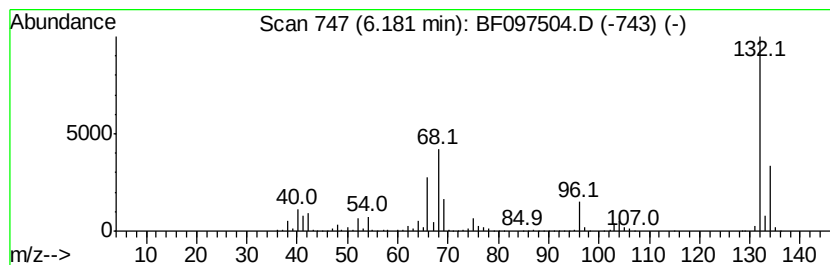
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Peak Number 3 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	90.13 ng	2577520	1,4-Dichlorobenzene-d4	6.40

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.82	2.7	ng	77767	1	6.40	571932	20.0
2-Pentanone, 4-hy...	4.55	32.7	ng	934045	1	6.40	571932	20.0
unknown6.18	6.18	90.1	ng	2577520	1	6.40	571932	20.0