LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108544.D
Acq On : 28 Aug 2018 7:18
Operator : JU/SJ
Sample : PB112391BL
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112391BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.396	5	10	15	rVB	56241	86406	2.46%	0.379%
2	5.248	490	495	503	rBV	119214	144211	4.11%	0.633%
3	5.631	556	560	573	rBV	2226088	2098108	59.82%	9.209%
4	6.619	723	728	731	rBV	2249962	2113022	60.25%	9.274%
5	6.772	749	754	757	rBV	2275530	2171935	61.93%	9.533%
6	6.995	789	792	796	rBV	702828	638937	18.22%	2.804%
7	7.154	815	819	823	rBV	2800889	2553918	72.82%	11.209%
8	7.560	883	888	892	rBV	1901506	2025225	57.75%	8.889%
9	8.283	1006	1011	1027	rBV	759618	742179	21.16%	3.258%
10	9.354	1188	1193	1196	rBV	3890167	3507136	100.00%	15.393%
11	10.042	1306	1310	1325	rVB2	825022	736584	21.00%	3.233%
12	10.836	1441	1445	1464	rBV	1232944	1193808	34.04%	5.240%
13	11.536	1560	1564	1572	rBV	754776	676446	19.29%	2.969%
14	12.918	1796	1799	1804	rBV	43948	37275	1.06%	0.164%
15	13.124	1829	1834	1837	rBV	3364091	2856109	81.44%	12.536%
16	14.189	2011	2015	2028	rBV	730593	693346	19.77%	3.043%
17	15.742	2273	2279	2289	rVB	360259	509019	14.51%	2.234%

Sum of corrected areas: 22783664

LSC Report - Integrated Chromatogram

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Instrument :
BNA_F
ClientSampleId :
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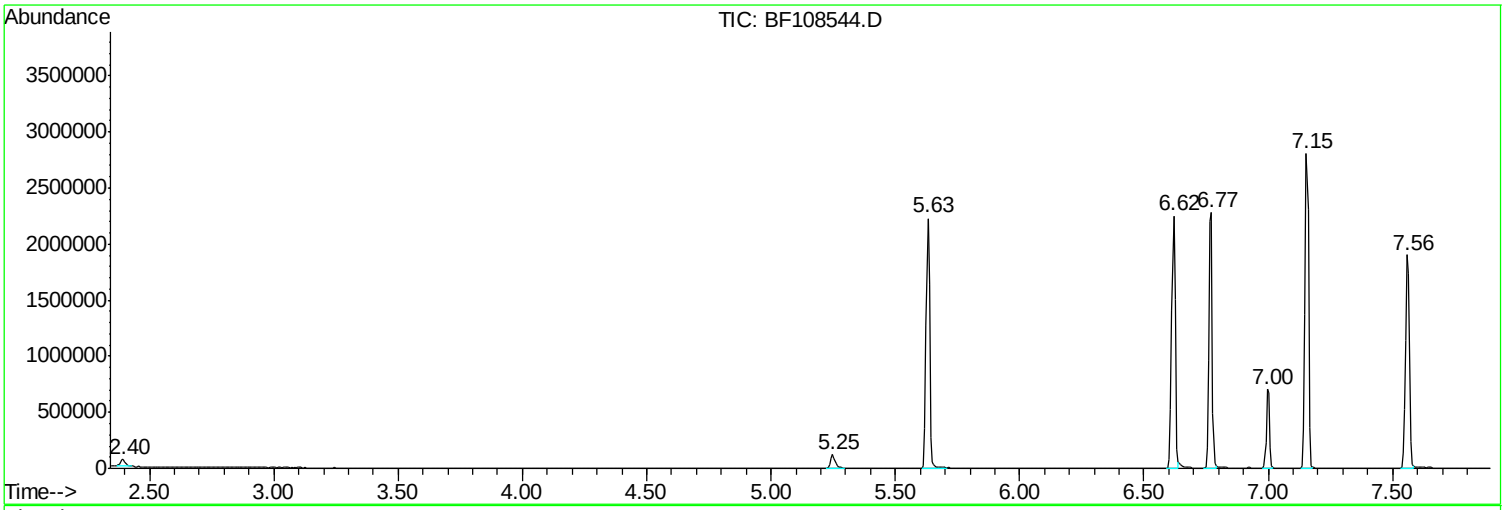
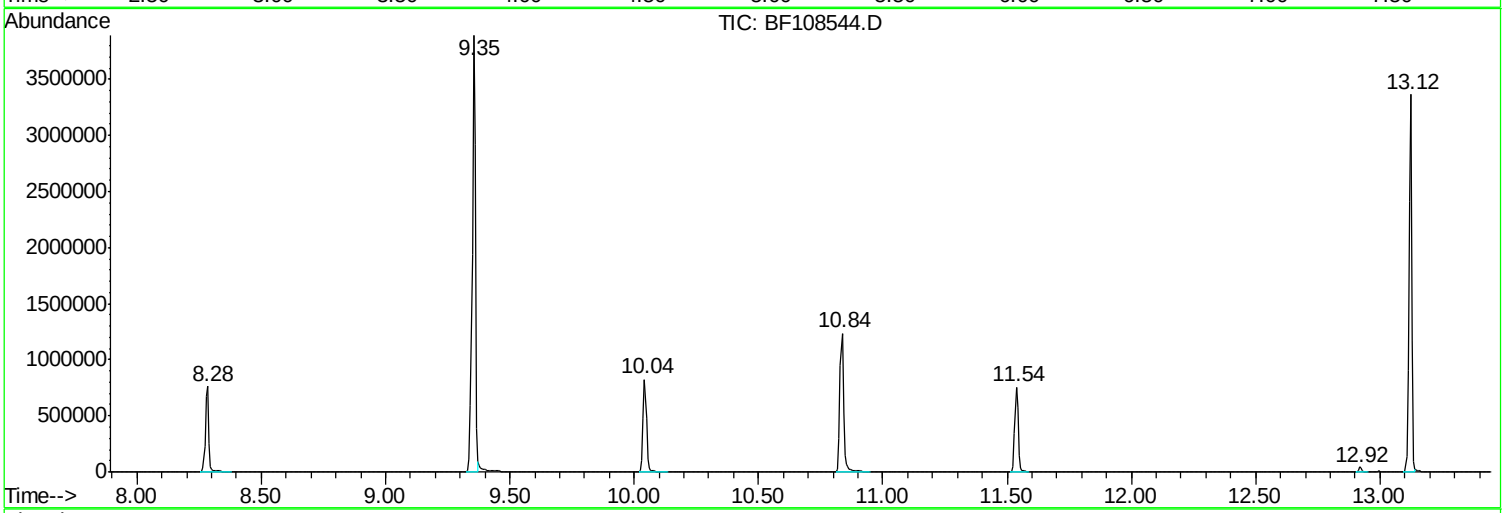
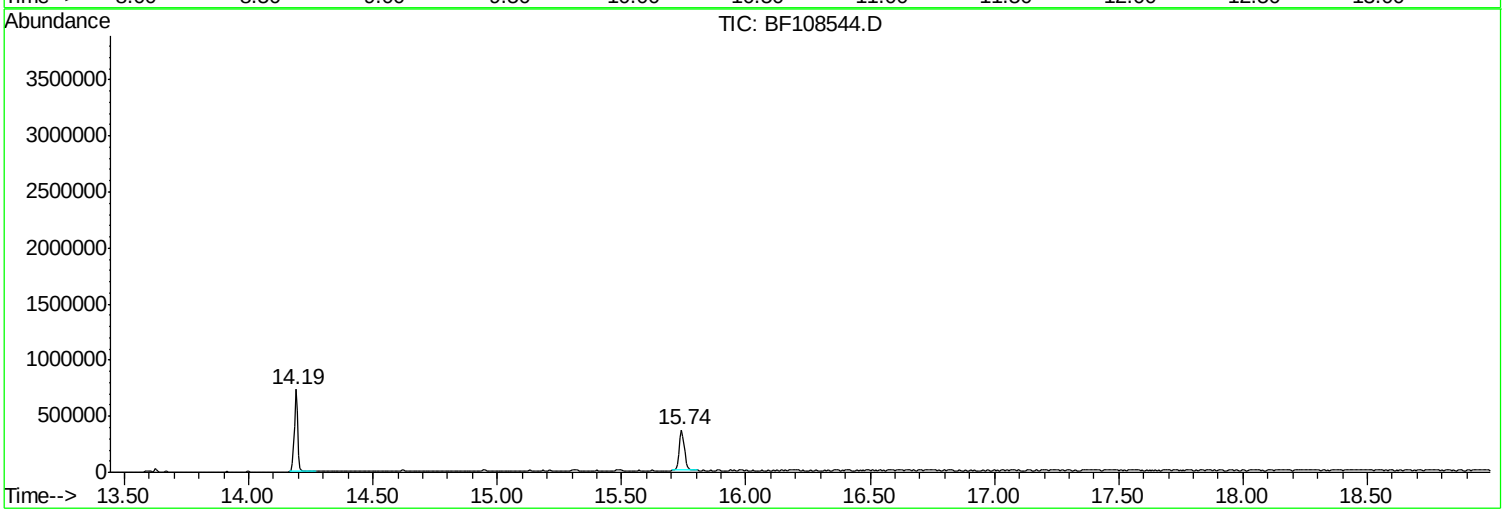
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Library Search Compound Report

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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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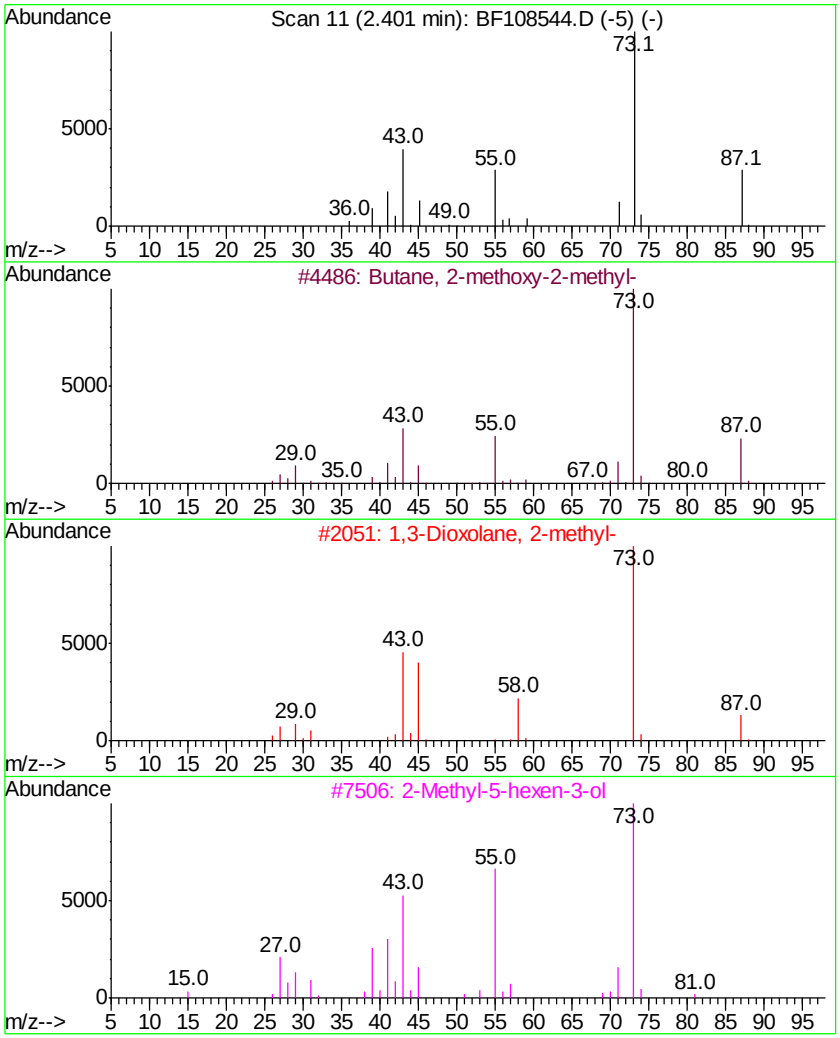
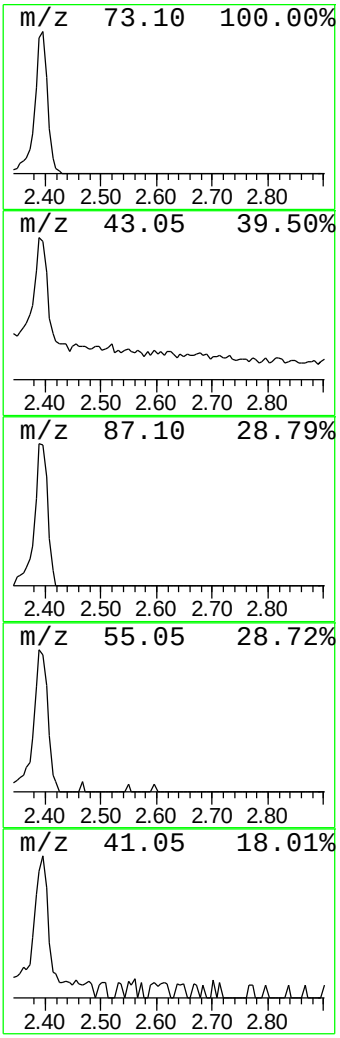
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	2.70 ng	86406	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9





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ClientSampleId :
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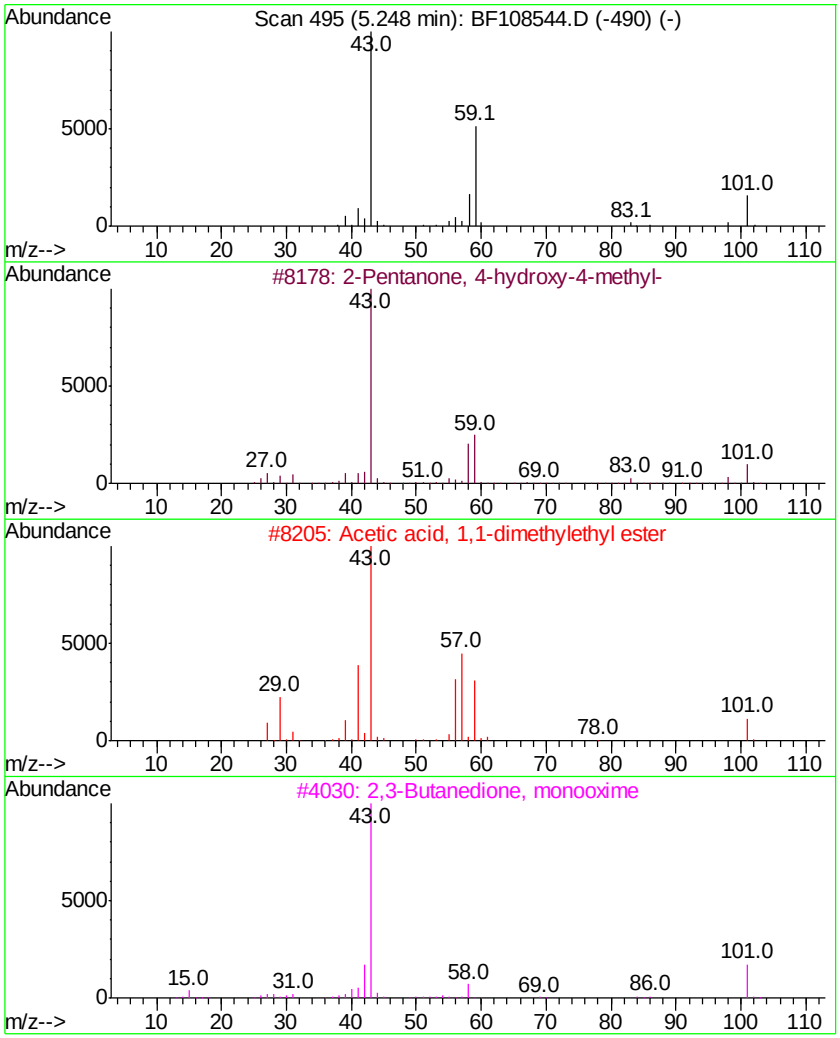
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

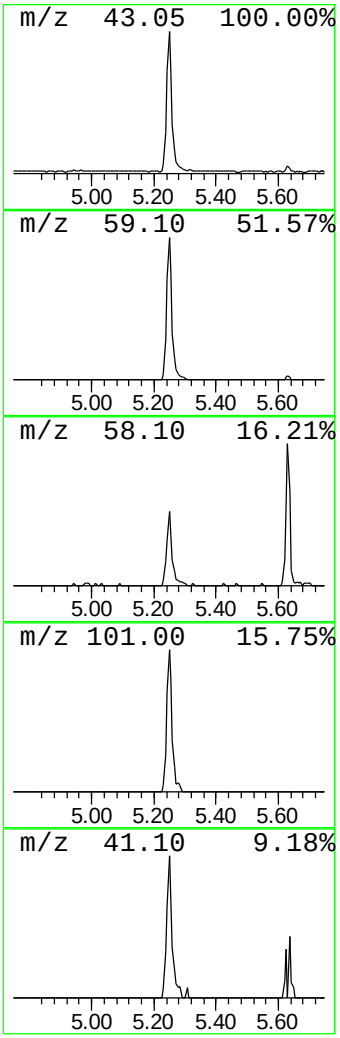
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	4.51 ng	144211	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





Library Search Compound Report

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BNA_F
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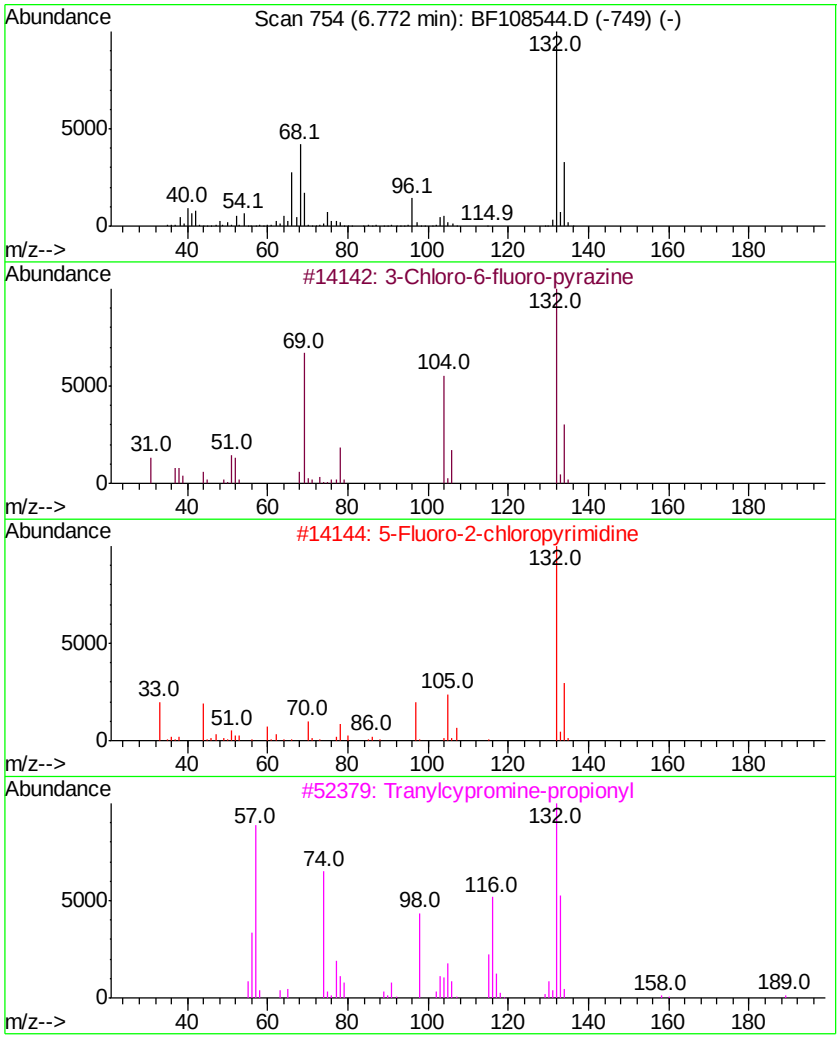
TIC Integration Parameters: LSCINT.P

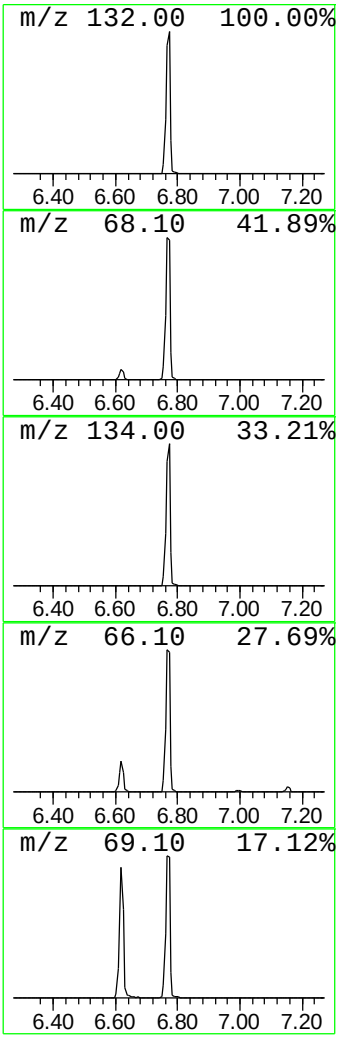
****

Peak Number 3 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	67.99 ng	2171940	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	2.40	2.7	ng	86406	1	7.00	638937	20.0
2-Pentanone, 4-hy...	5.25	4.5	ng	144211	1	7.00	638937	20.0
unknown6.77	6.77	68.0	ng	2171940	1	7.00	638937	20.0