

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
 Data File : BF137394.D
 Acq On : 26 Feb 2024 19:32
 Operator : CG\JU
 Sample : P1538-14
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20241107-AMENDED-COMPOSITE-35N-N-4-06

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-BF022324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	492	511	514	rBV	8542701	33658707	100.00%	55.009%
2	5.422	563	567	591	rVB	1640423	1615843	4.80%	2.641%
3	6.416	732	736	749	rBV	3030715	3038562	9.03%	4.966%
4	6.781	795	798	806	rBV	1490597	1265948	3.76%	2.069%
5	7.345	889	894	908	rBV	3471631	3640394	10.82%	5.950%
6	7.498	916	920	924	rBV	965721	866247	2.57%	1.416%
7	8.057	1012	1015	1033	rVB	1927488	1726241	5.13%	2.821%
8	9.139	1194	1199	1202	rBV	6019984	5285546	15.70%	8.638%
9	9.816	1310	1314	1317	rVB	2022633	1657336	4.92%	2.709%
10	10.604	1445	1448	1456	rBV	643482	563024	1.67%	0.920%
11	10.728	1466	1469	1477	rBV	345978	380073	1.13%	0.621%
12	11.304	1564	1567	1570	rBV	1487341	1367788	4.06%	2.235%
13	12.910	1836	1840	1843	rBV	3965227	3759311	11.17%	6.144%
14	13.957	2015	2018	2022	rBV	1120337	1180597	3.51%	1.929%
15	15.439	2266	2270	2279	rVV	871159	1181649	3.51%	1.931%

Sum of corrected areas: 61187266

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137394.D
Acq On : 26 Feb 2024 19:32
Operator : CG\JU
Sample : P1538-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :

BNA_F

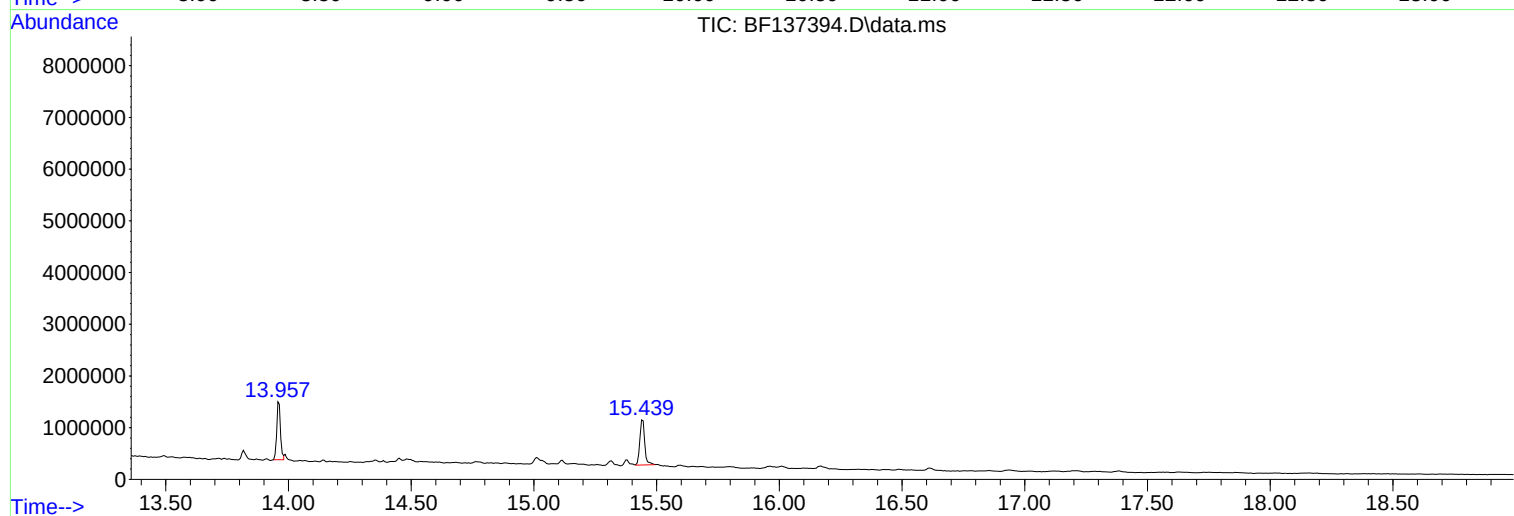
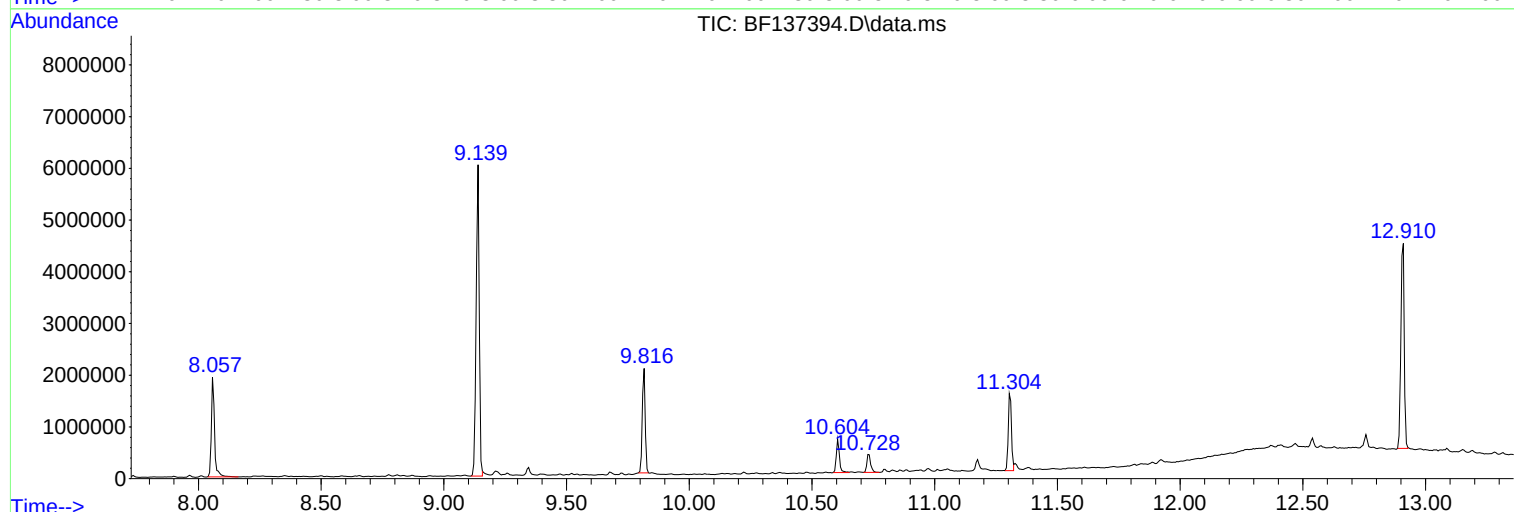
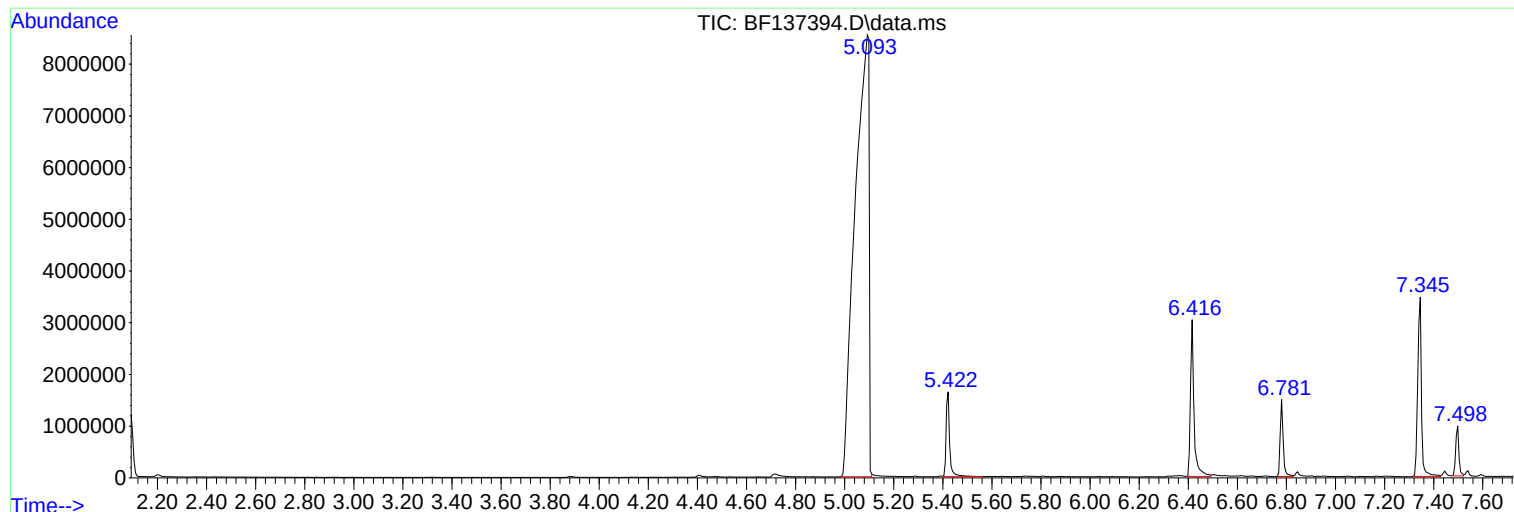
ClientSampleId :

20241107-AMENDED-COMPOSITE-35N-N-4-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137394.D
Acq On : 26 Feb 2024 19:32
Operator : CG\JU
Sample : P1538-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241107-AMENDED-COMPOSITE-35N-N-4-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

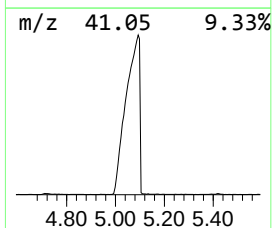
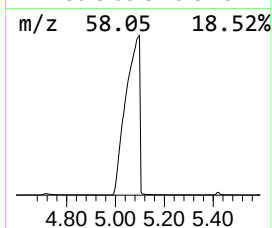
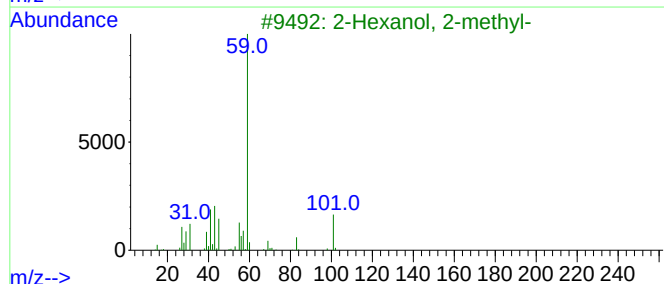
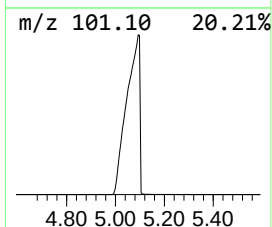
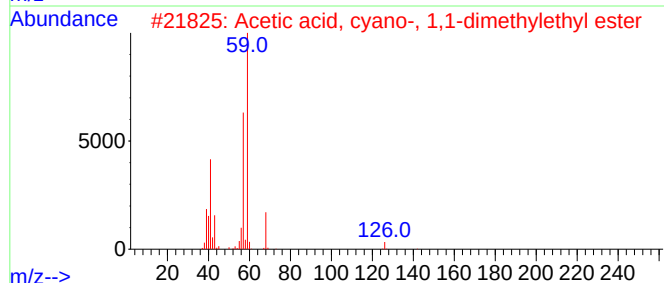
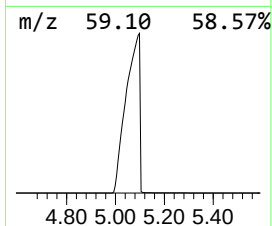
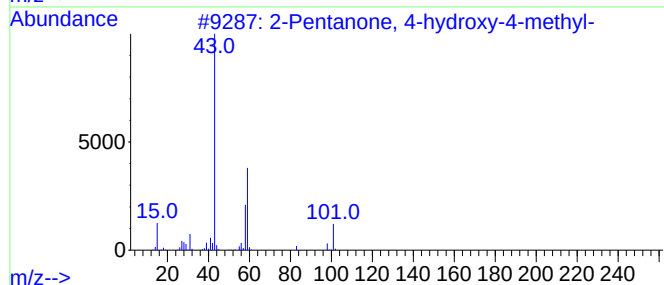
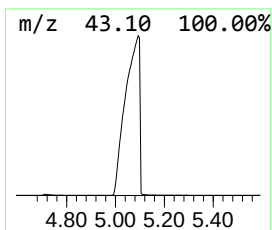
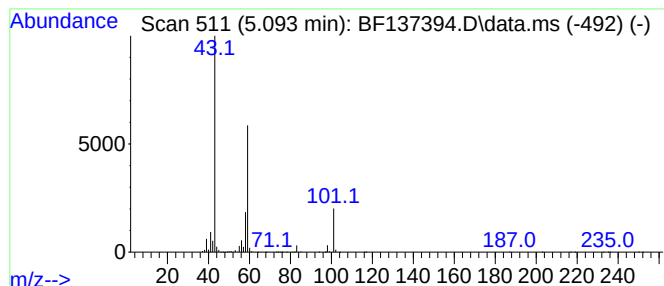
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	531.76 ng	33658700	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
5	Acetone	58	C3H6O	000067-64-1	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137394.D
Acq On : 26 Feb 2024 19:32
Operator : CG\JU
Sample : P1538-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241107-AMENDED-COMPOSITE-35N-N-4-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

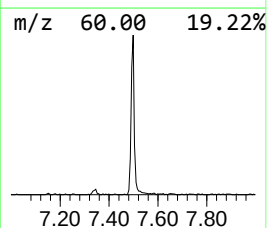
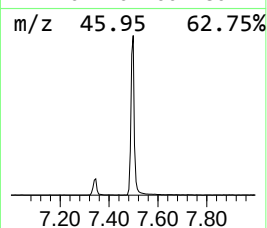
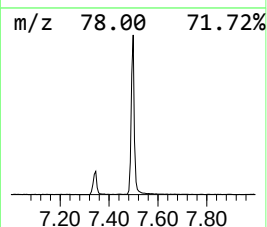
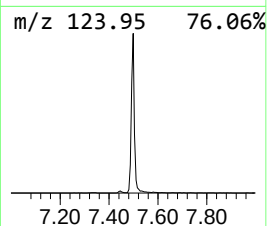
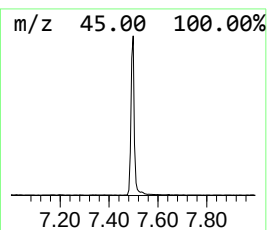
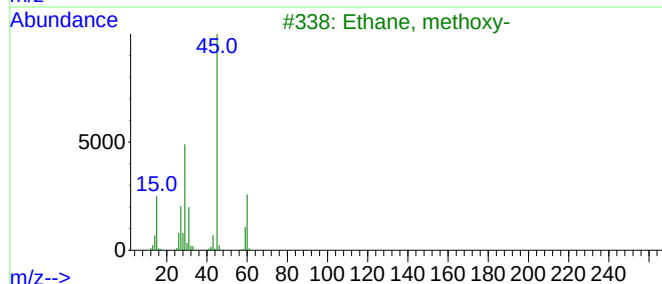
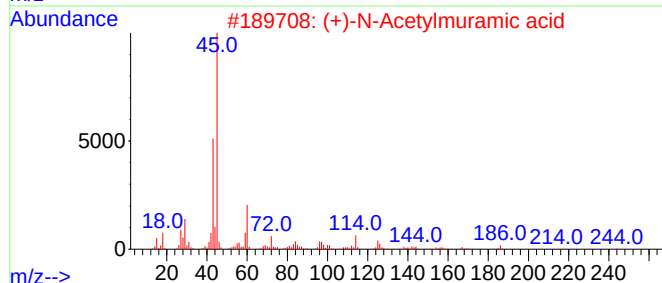
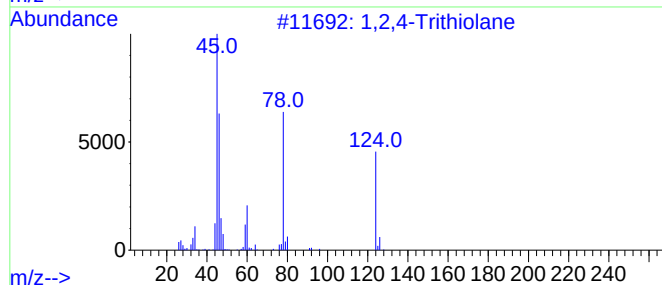
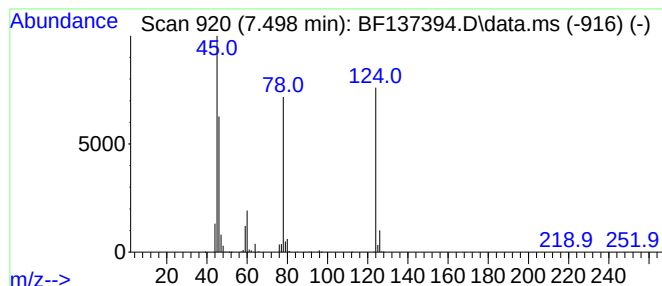
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.498	10.04 ng	866247	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	94
2			(+)-N-Acetylmuramic acid	293	C11H19NO8	010597-89-4	12
3			Ethane, methoxy-	60	C3H8O	000540-67-0	9
4			Dimethyl ether	46	C2H6O	000115-10-6	9
5			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137394.D
Acq On : 26 Feb 2024 19:32
Operator : CG\JU
Sample : P1538-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241107-AMENDED-COMPOSITE-35N-N-4-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

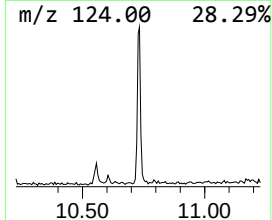
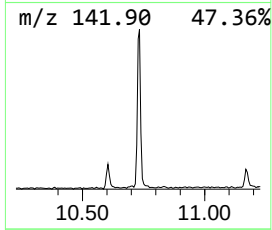
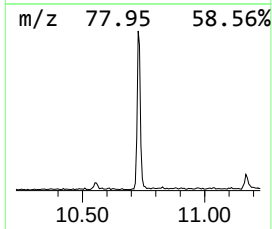
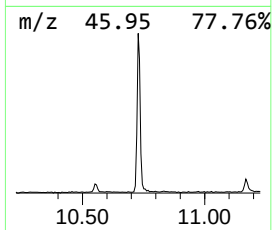
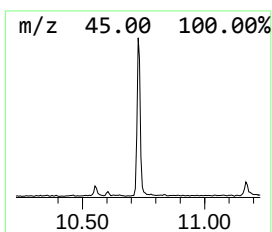
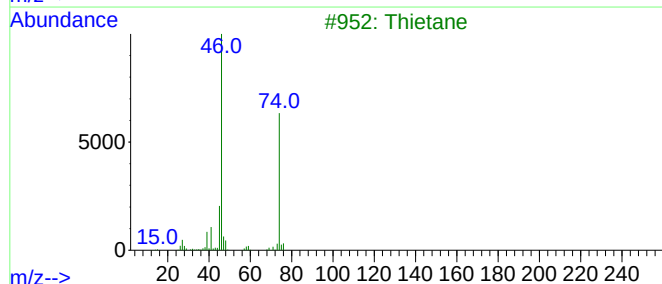
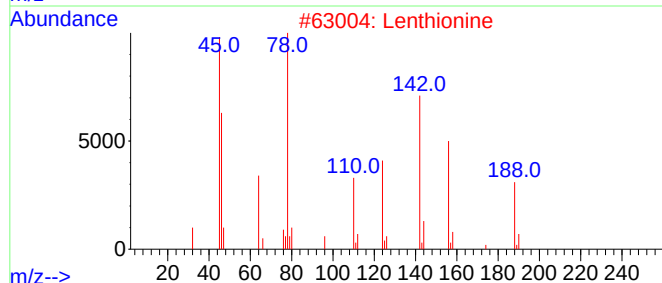
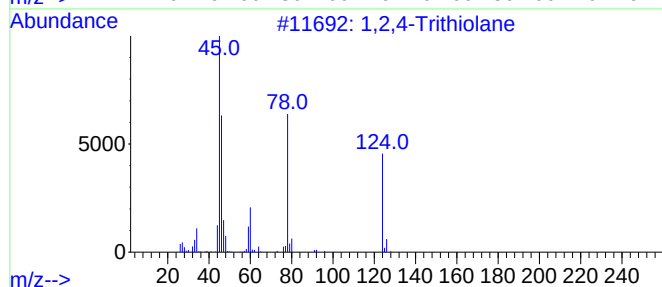
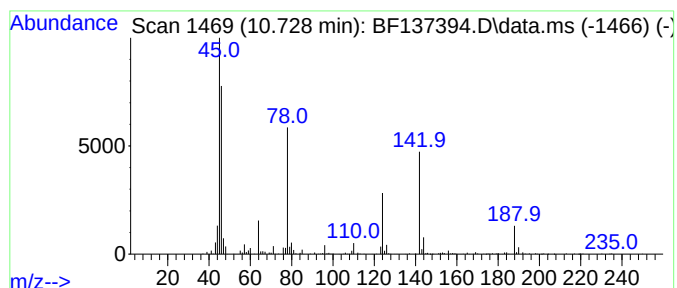
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.727

Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.727	5.56 ng	380073	Phenanthrene-d10	11.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
2	Lenthionine	188	C2H4S5	000292-46-6	38
3	Thietane	74	C3H6S	000287-27-4	25
4	Methanesulfinothioic acid, S-1-p...	138	C4H10OS2	1000322-32-0	17
5	1,3-Dithiane-4,6-dione	148	C4H4O2S2	052133-76-3	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137394.D
Acq On : 26 Feb 2024 19:32
Operator : CG\JU
Sample : P1538-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241107-AMENDED-COMPOSITE-35N-N-4-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.093	531.8	ng	33658700	1	6.781	1265950	20.0
1,2,4-Trithiolane	7.498	10.0	ng	866247	2	8.057	1726240	20.0
unknown10.727	10.727	5.6	ng	380073	4	11.304	1367790	20.0