LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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: BF137432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	11	rVB	4671615	7199521	99.53%	13.025%
2	3.263	195	200	214	rVB	67197	143157	1.98%	0.259%
3	3.587	250	255	265	rVB2	165383	309039	4.27%	0.559%
4	3.881	298	305	314	rVB2	125995	237010	3.28%	0.429%
5	3.957	314	318	320	rBV	176858	235971	3.26%	0.427%
6	3.981	320	322	329	rVB	206002	295812	4.09%	0.535%
7	4.157	347	352	362	rBV	134393	212516	2.94%	0.384%
8	4.416	392	396	409	rVB	256643	338076	4.67%	0.612%
9	4.528	410	415	418	rVV	132567	156485	2.16%	0.283%
10	4.575	418	423	437	rVB	1188854	1391339	19.23%	2.517%
11	4.740	446	451	455	rBV	565169	709363	9.81%	1.283%
12	4.781	455	458	467	rVB2	66028	88790	1.23%	0.161%
13	5.016	489	498	501	rBV	4657235	7233592	100.00%	13.087%
14	5.110	511	514	520	rBV	60567	75012	1.04%	0.136%
15	5.410	561	565	571	rBV	1143217	1160503	16.04%	2.100%
16	5.593	593	596	600	rBV	146224	140256	1.94%	0.254%
17	5.798	627	631	635	rBV	92539	77354	1.07%	0.140%
18	5.875	640	644	647	rBV2	108242	133513	1.85%	0.242%
19	5.904	647	649	654	rVB2	97381	94617	1.31%	0.171%
20	6.157	688	692	694	rBV	98620	98425	1.36%	0.178%
21	6.181	694	696	699	rVV2	101705	101194	1.40%	0.183%
22	6.210	699	701	710	rVB2	122279	163228	2.26%	0.295%
23	6.387	729	731	733	rBV	110774	91762	1.27%	0.166%
24	6.416	733	736	747	rVB	2662157	2362005	32.65%	4.273%
25	6.657	775	777	786	rBV	221944	244483	3.38%	0.442%
26	6.781	792	798	804	rBV	931018	871102	12.04%	1.576%
27	6.869	810	813	817	rVB	113378	99025	1.37%	0.179%
28	6.904	817	819	823	rBV2	151564	149193	2.06%	0.270%
29	7.345	890	894	903	rBV	2302155	2334635	32.27%	4.224%
30	7.504	916	921	925	rVV	5111348	6206000	85.79%	11.228%
31	7.534	925	926	934	rVB2	82893	121692	1.68%	0.220%
32	8.004	1002	1006	1010	rVB	127417	123197	1.70%	0.223%
33	8.057	1012	1015	1025	rBV	1218580	1142054	15.79%	2.066%
34	8.139	1026	1029	1036	rVB2	114666	134162	1.85%	0.243%
35	8.222	1039	1043	1045	rBV	188453	183693	2.54%	0.332%
36	8.345	1059	1064	1066	rVV2	154564	218849	3.03%	0.396%

LSC Area Percent Report

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Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

37	8.369	1066	1068	1072	rVV2	167638	183551	2.54%	0.332%
38	8.404	1072	1074	1077	rVB	123837	88198	1.22%	0.160%
39	9.139	1195	1199	1202	rBV	5236607	4324195	59.78%	7.823%
40	9.210	1207	1211	1216	rVV	568608	537239	7.43%	0.972%
41	9.345	1231	1234	1243	rBV	409584	398068	5.50%	0.720%
42	9.786	1305	1309	1311	rBV	99339	126068	1.74%	0.228%
43	9.816	1311	1314	1318	rVB	1822787	1459163	20.17%	2.640%
44	10.128	1363	1367	1376	rBV	166845	193448	2.67%	0.350%
45	10.557	1434	1440	1445	rBV4	58424	84696	1.17%	0.153%
46	10.610	1445	1449	1457	rVV	648593	609534	8.43%	1.103%
47	10.739	1467	1471	1478	rBV	1482162	1424654	19.69%	2.577%
48	11.180	1542	1546	1555	rVB	291992	331578	4.58%	0.600%
49	11.310	1564	1568	1576	rBV	1911145	1706405	23.59%	3.087%
50	12.533	1773	1776	1779	rBV	110322	89712	1.24%	0.162%
51	12.757	1811	1814	1817	rBV	108351	108236	1.50%	0.196%
52	12.916	1836	1841	1844	rBV	5472620	5198852	71.87%	9.406%
53	13.651	1963	1966	1973	rVB	85780	102781	1.42%	0.186%
54	13.821	1992	1995	2002	rBV	369675	462718	6.40%	0.837%
55	13.969	2016	2020	2033	rVB	1521006	1544024	21.35%	2.793%
56	14.457	2100	2103	2107	rBV	92475	110614	1.53%	0.200%
57	15.027	2196	2200	2207	rVB	41542	84939	1.17%	0.154%
58	15.121	2213	2216	2220	rVB2	79112	83372	1.15%	0.151%
59	15.457	2268	2273	2280	rBV	872154	1144267	15.82%	2.070%

Sum of corrected areas: 55272937

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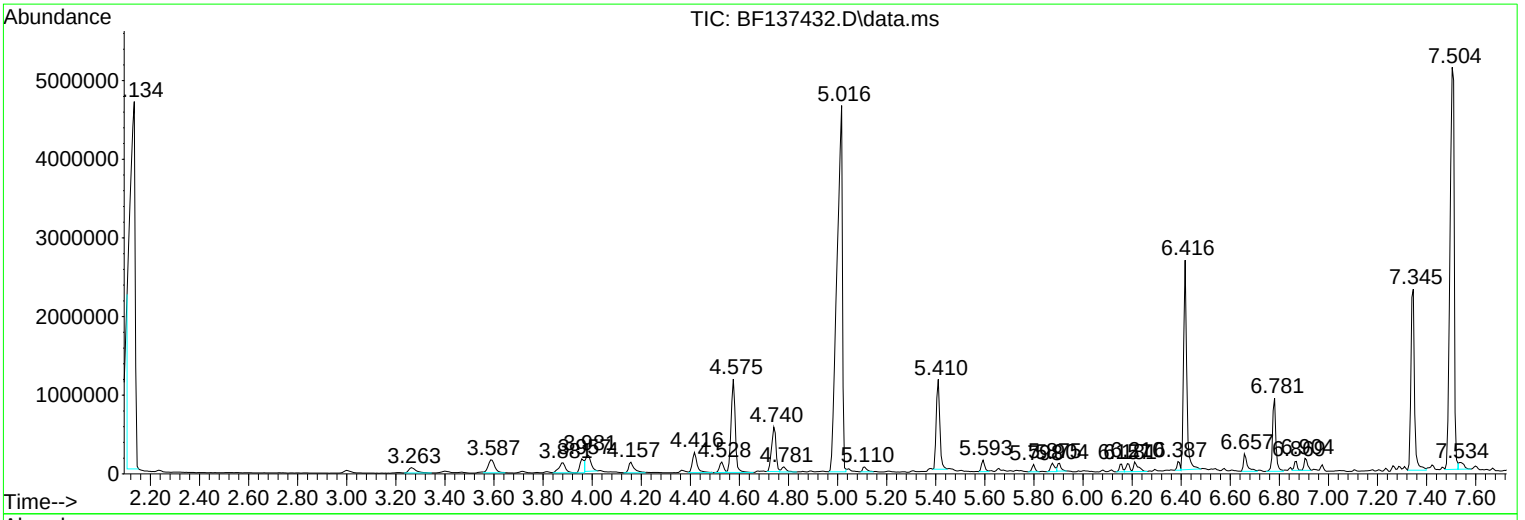
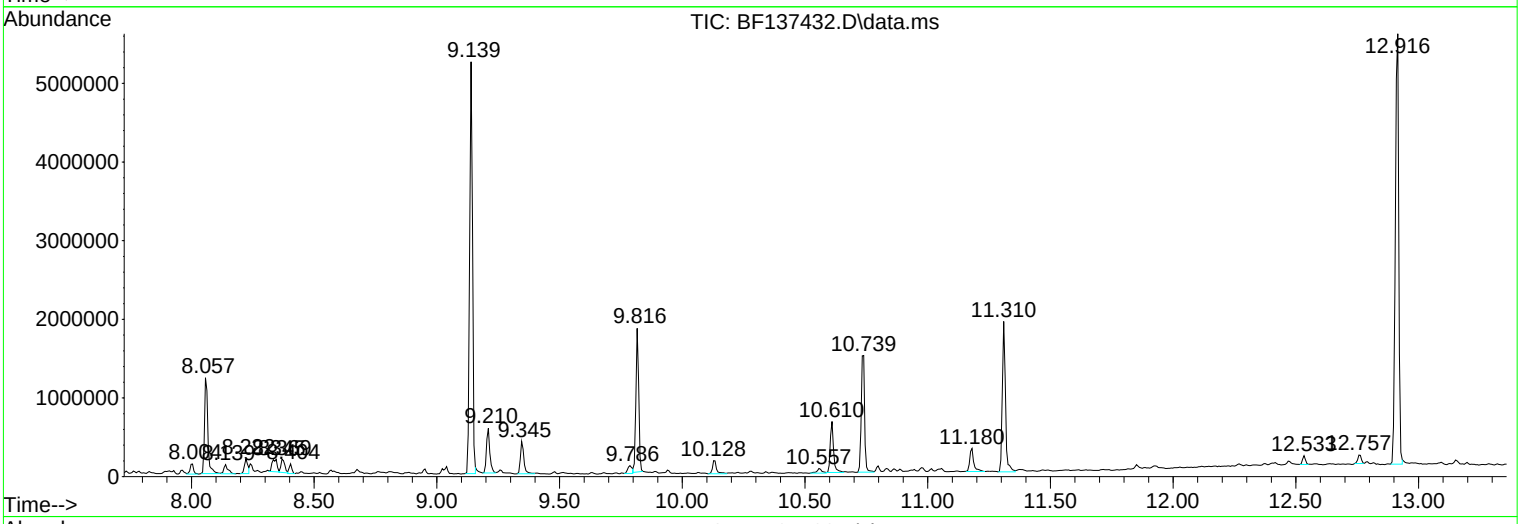
Misc :
ALS Vial : 13 Sample Multiplier: 1

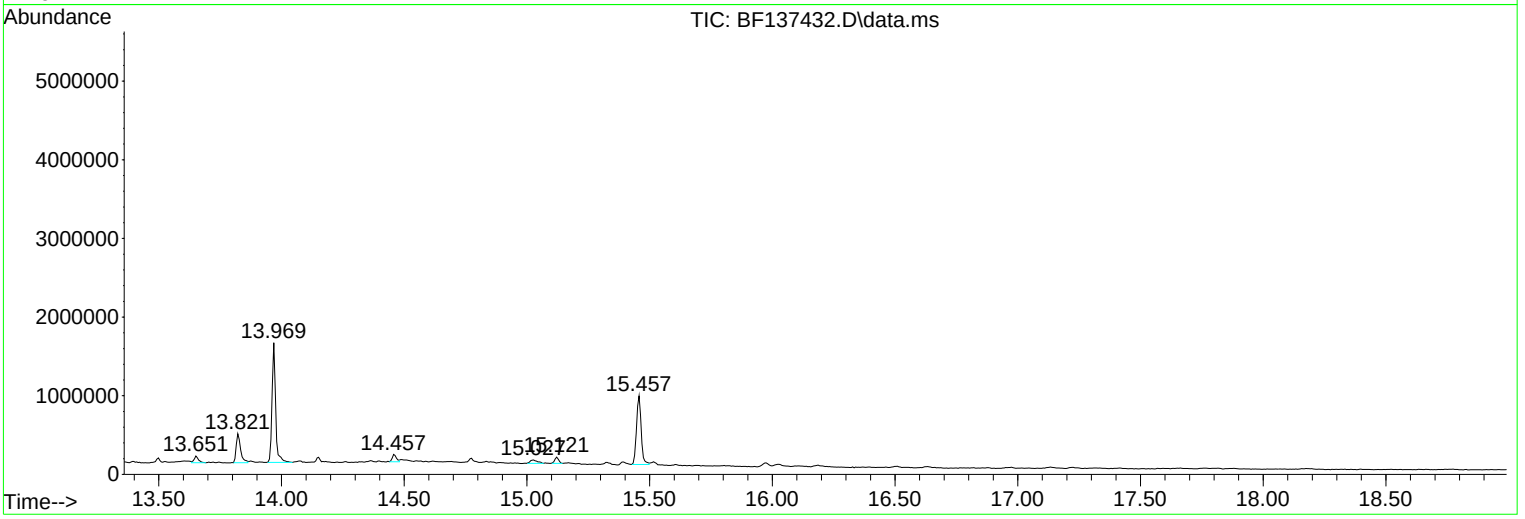
Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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\BF022824\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

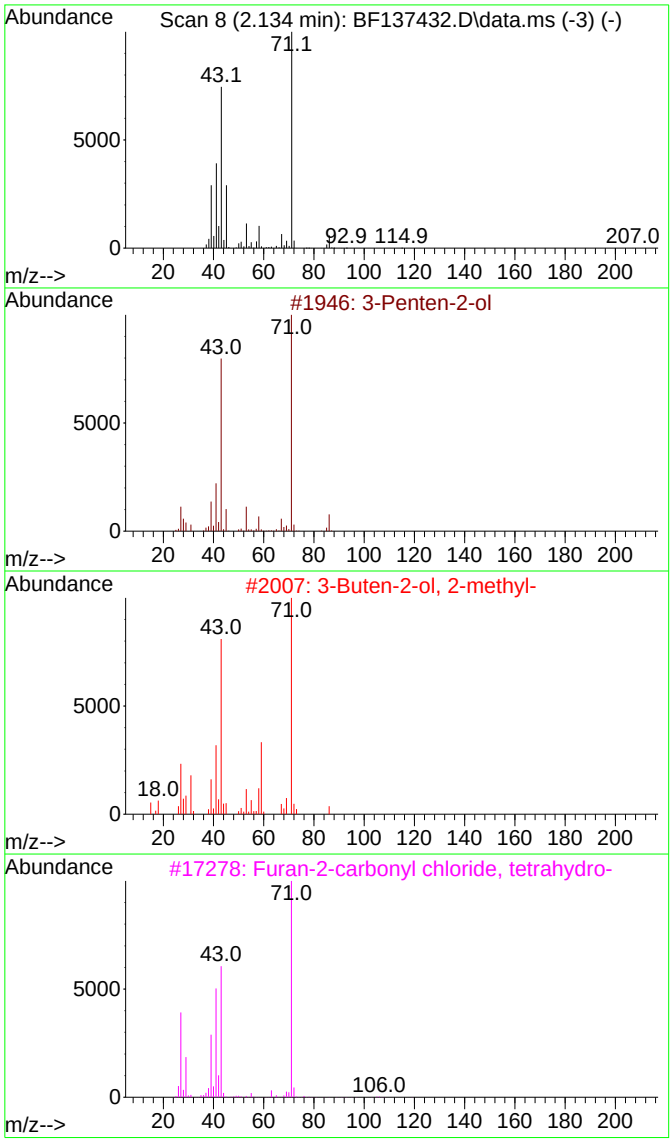
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

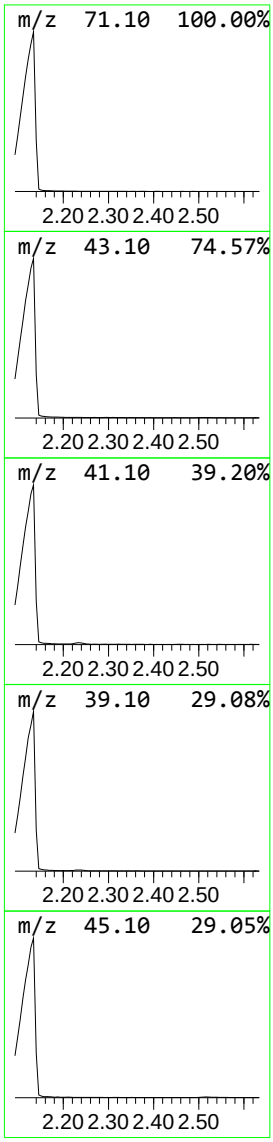
****

Peak Number 1 3-Penten-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	165.30 ng	7199520	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	83
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
3	Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	53
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	45
5	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
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Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

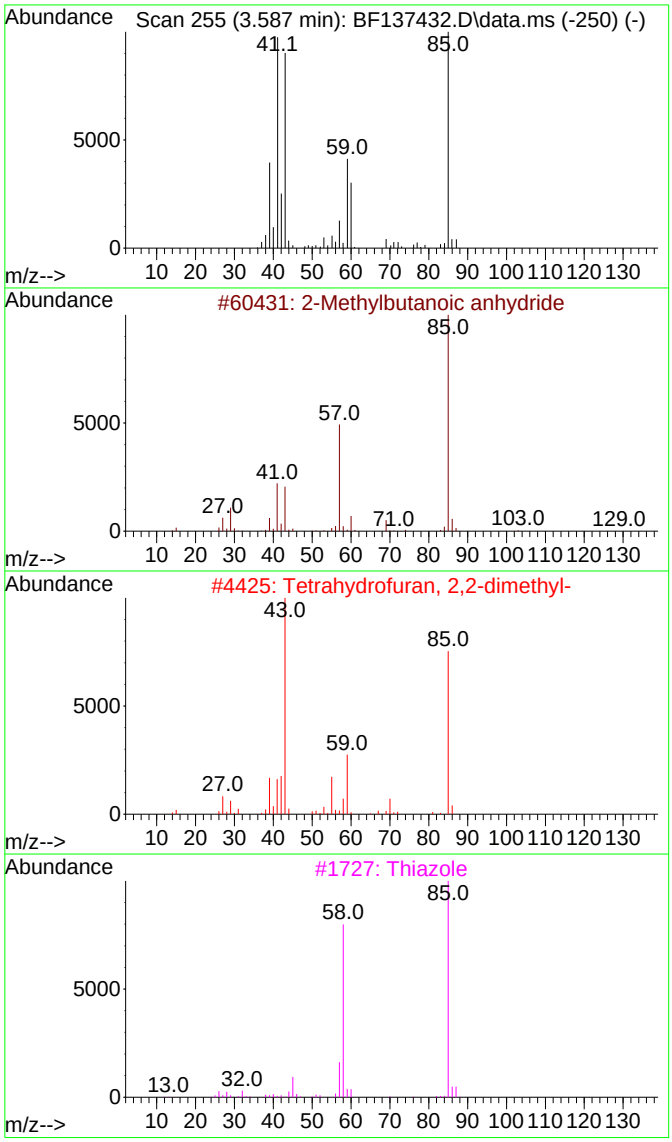
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

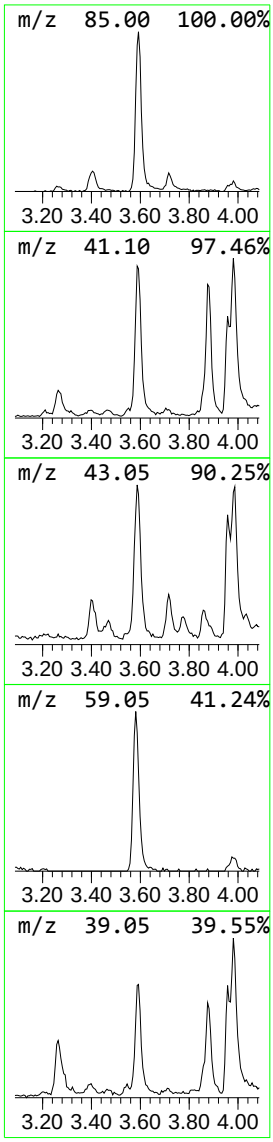
****

Peak Number 2 unknown3.587 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.587	7.10 ng	309039	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	38
2	Tetrahydrofuran, 2,2-dimethyl-	100	C6H12O	001003-17-4	37
3	Thiazole	85	C3H3NS	000288-47-1	35
4	Sulfurous acid, isohexyl 2-propy...	208	C9H20O3S	1000309-11-6	27
5	1,5-Heptadien-4-ol, 3,3,6-trimet...	154	C10H18O	027644-04-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
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Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

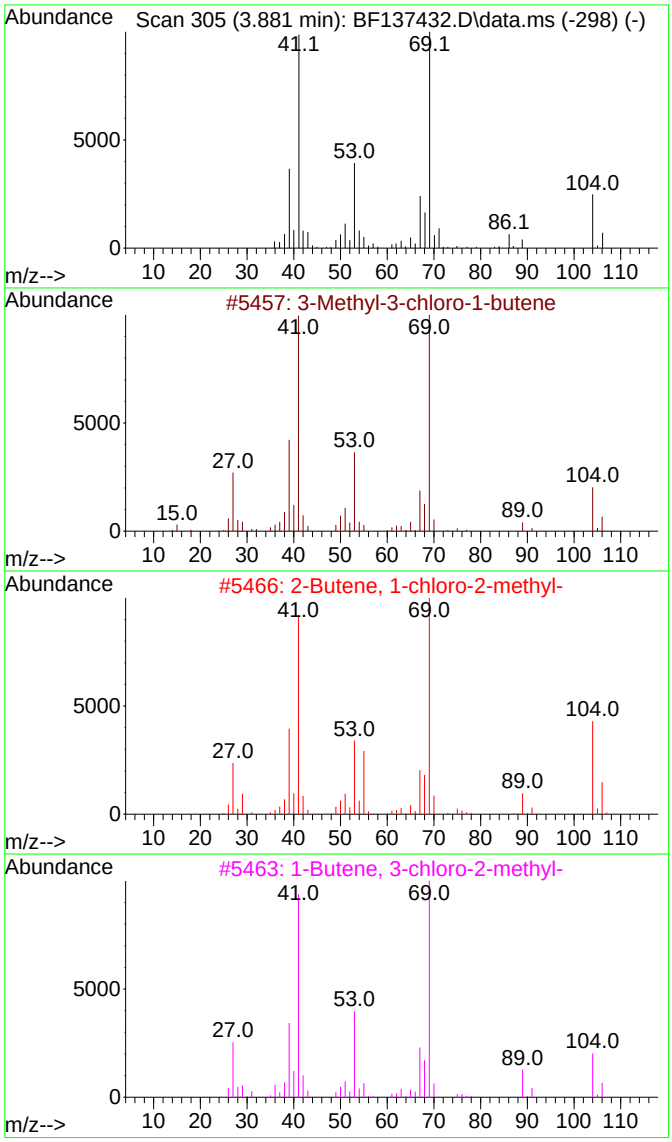
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

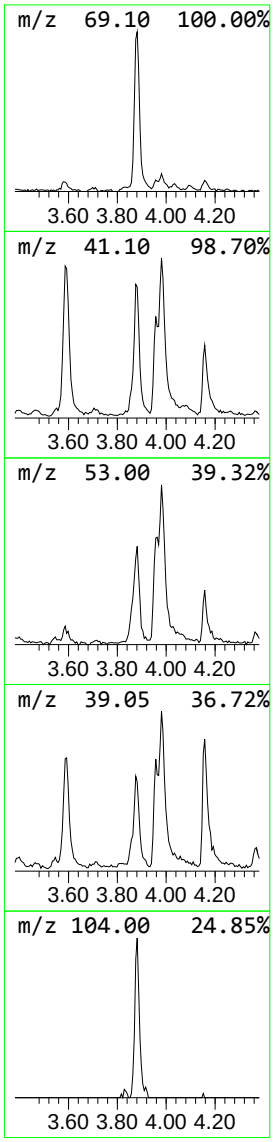
****

Peak Number 3 3-Methyl-3-chloro-1-butene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.881	5.44 ng	237010	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	91
2	2-Butene, 1-chloro-2-methyl-	104	C5H9Cl	013417-43-1	90
3	1-Butene, 3-chloro-2-methyl-	104	C5H9Cl	005166-35-8	87
4	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	78
5	2-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-65-8	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
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Instrument :
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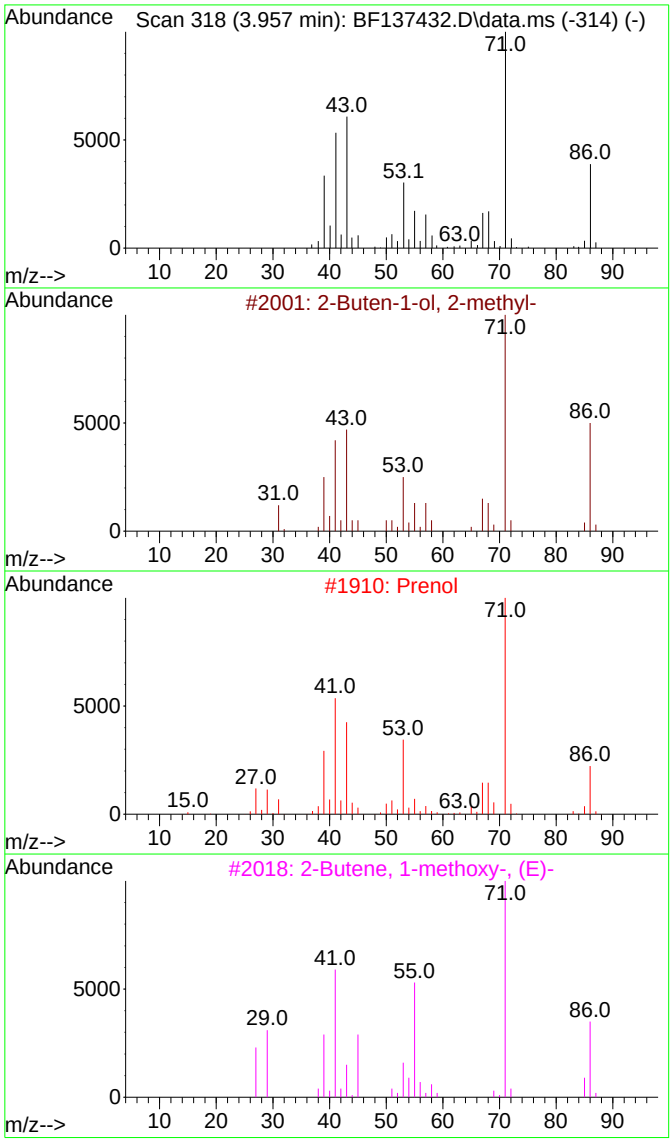
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

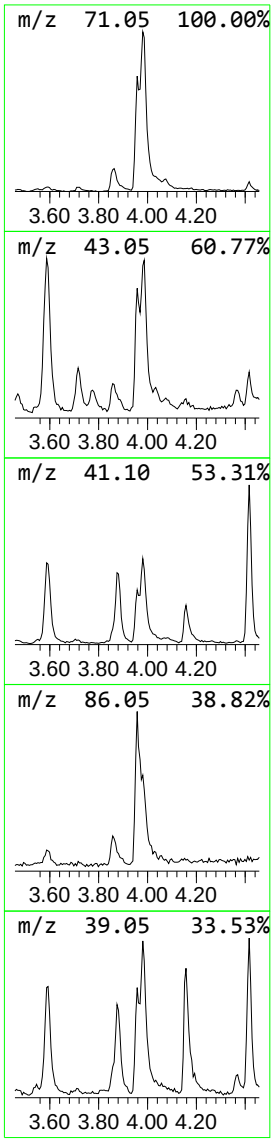
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Buten-1-ol, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.957	5.42 ng	235971	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	91
2	Prenol	86	C5H10O	000556-82-1	78
3	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	59
4	Acetaldehyde, ethylhydrazone	86	C4H10N2	020487-02-9	59
5	(Z)-CH3CH2CH=CH(OCH3)	86	C5H10O	010034-12-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
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Instrument :
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ClientSampleId :
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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

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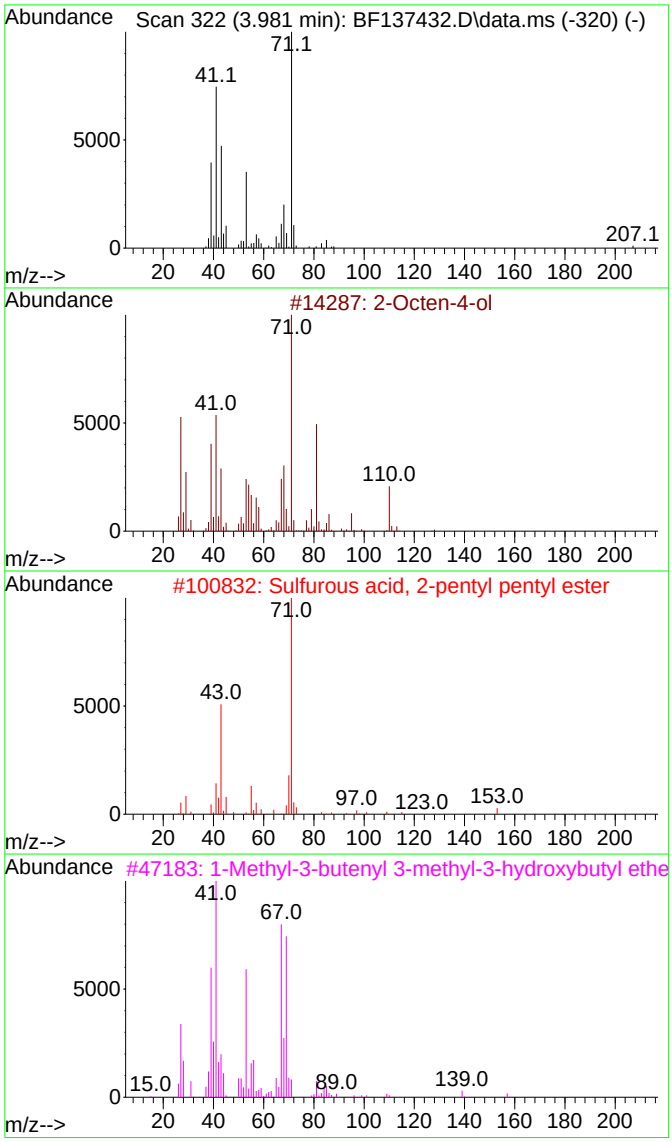
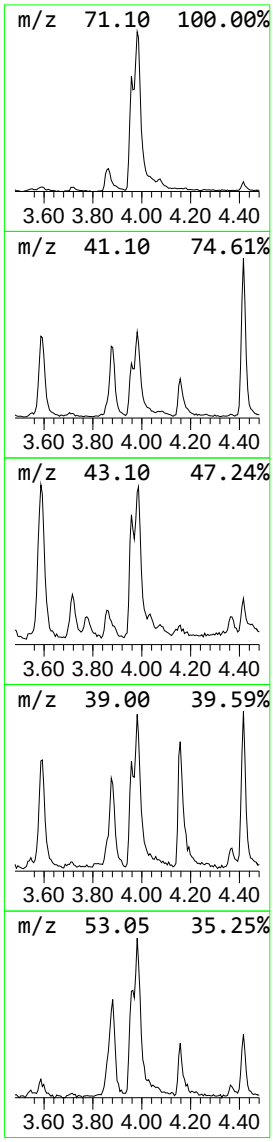
Peak Number 5 unknown3.981 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	6.79 ng	295812	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octen-4-ol	128	C8H16O	004798-61-2	36
2	Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	35
3	1-Methyl-3-butenyl 3-methyl-3-hy...	172	C10H20O2	1010139-77-4	25
4	1,7-Octadiene, 3-methoxy-	140	C9H16O	020202-62-4	23
5	4-Hexen-3-ol	100	C6H12O	004798-58-7	23





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Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

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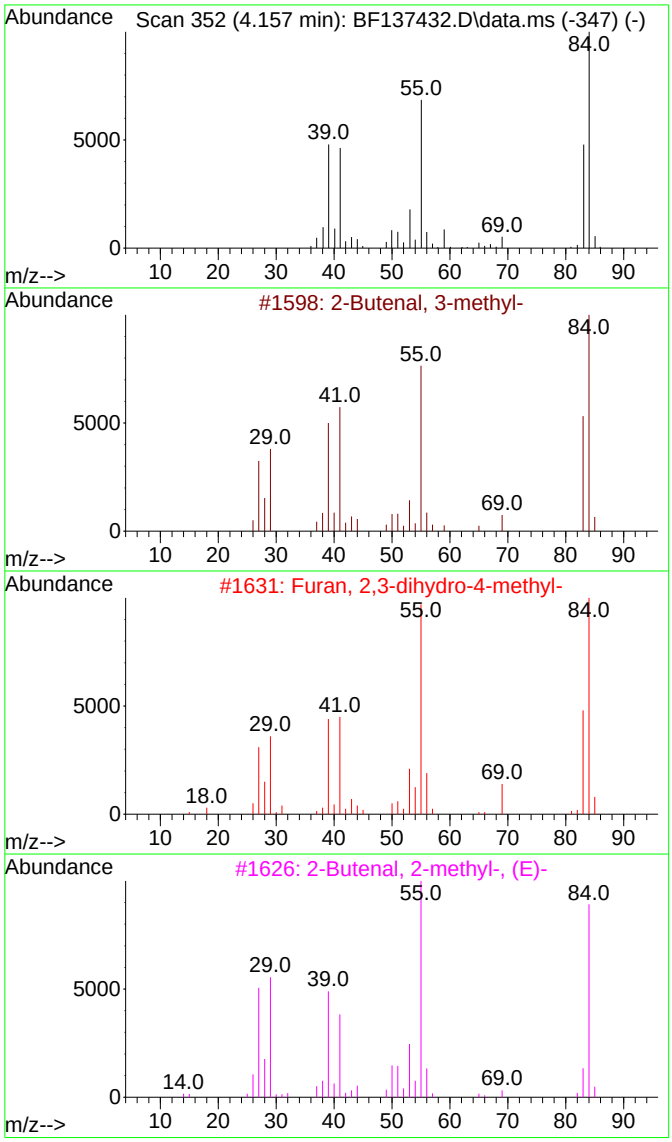
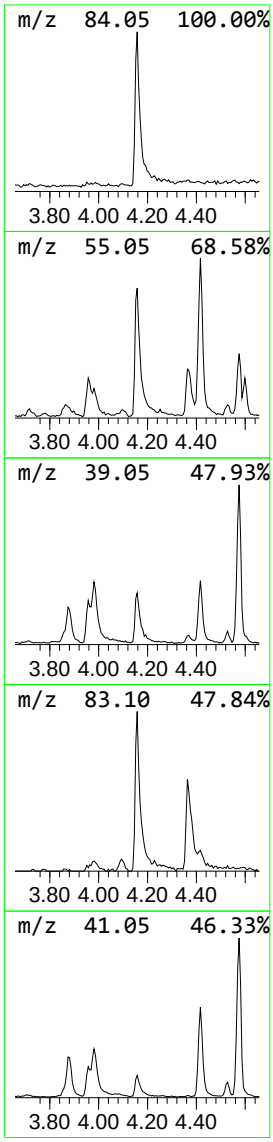
Peak Number 6 2-Butenal, 3-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.157	4.88 ng	212516	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	93
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	72
3	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	47
4	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	47
5	2-Ethylacrolein	84	C5H8O	000922-63-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

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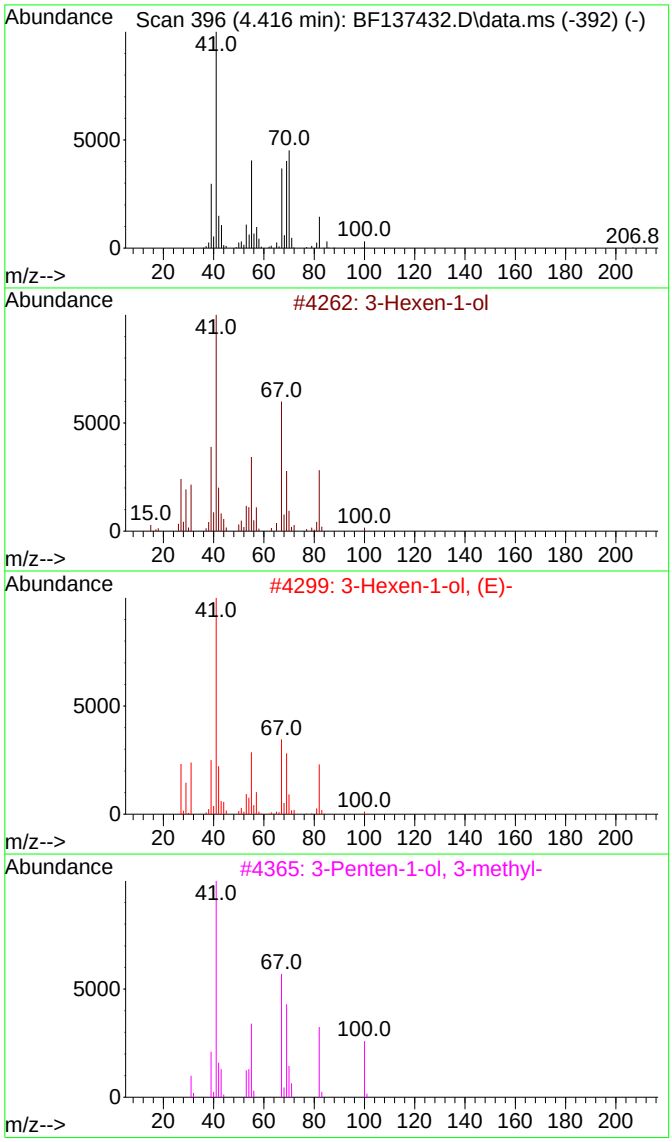
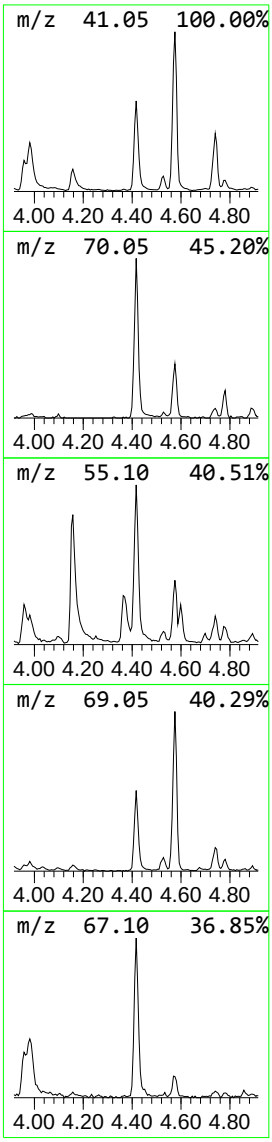
Peak Number 7 unknown4.416 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	7.76 ng	338076	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-1-ol	100	C6H12O	000544-12-7	47
2	3-Hexen-1-ol, (E)-	100	C6H12O	000928-97-2	47
3	3-Penten-1-ol, 3-methyl-	100	C6H12O	001708-99-2	47
4	2-Hexene, 3,5-dimethyl-	112	C8H16	003404-79-3	42
5	3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	37





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Sample : P1523-08
Misc :
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ClientSampleId :
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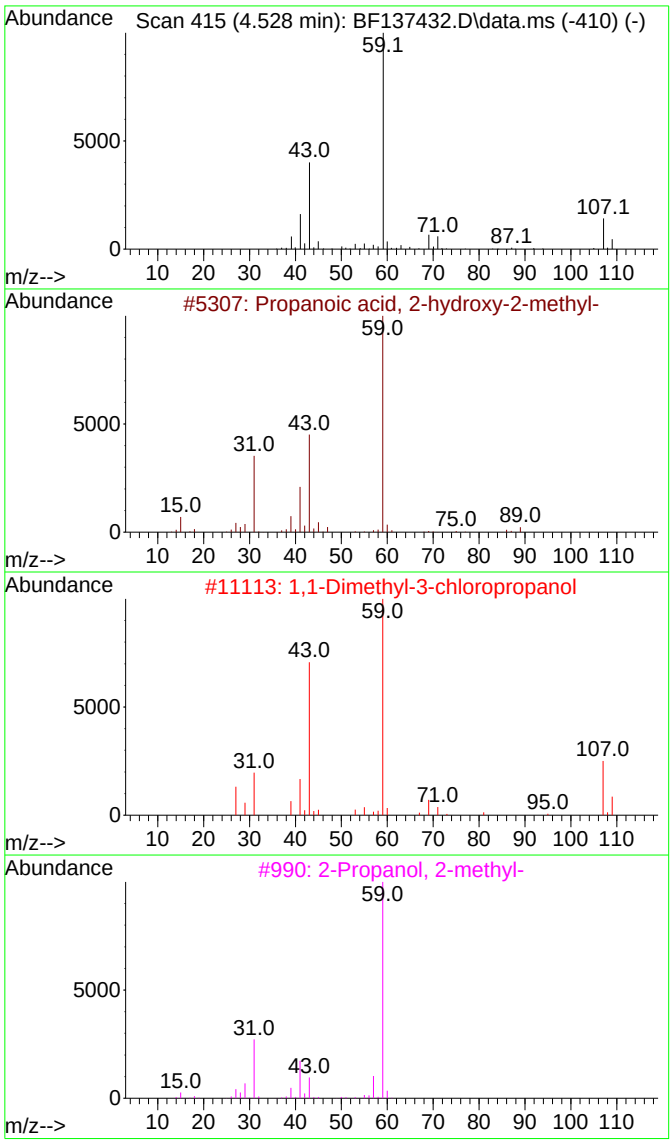
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

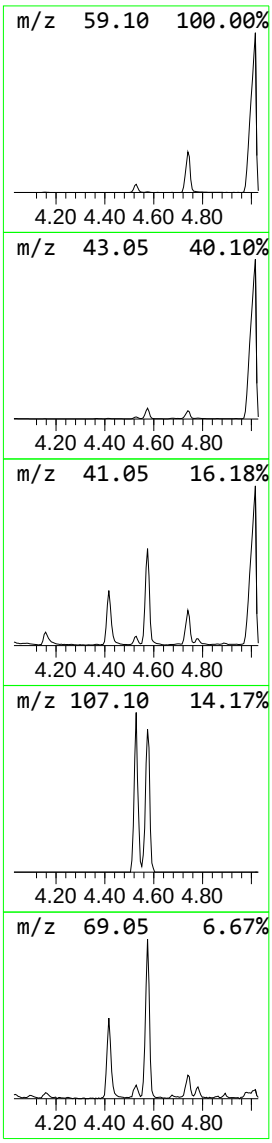
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Propanoic acid, 2-hydroxy-2... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.528	3.59 ng	156485	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	59
2	1,1-Dimethyl-3-chloropropanol	122	C5H11ClO	001985-88-2	56
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40
4	3-Pentanol	88	C5H12O	000584-02-1	36
5	4-Methyl-2-pentanol, methyl ether	116	C7H16O	1000333-93-5	36





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

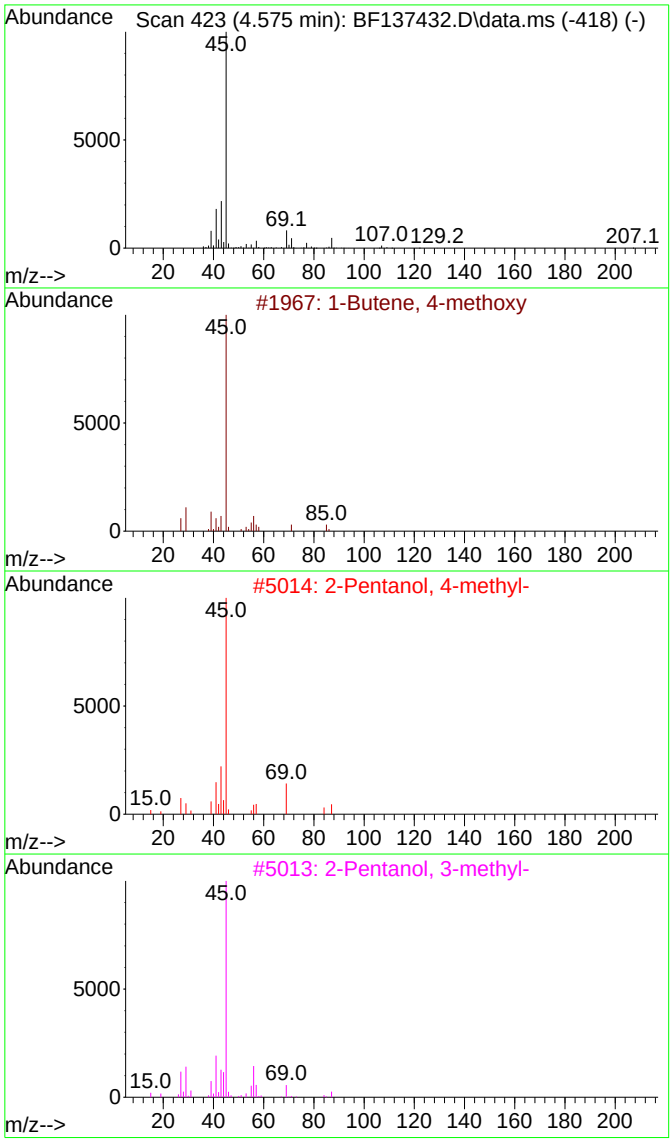
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

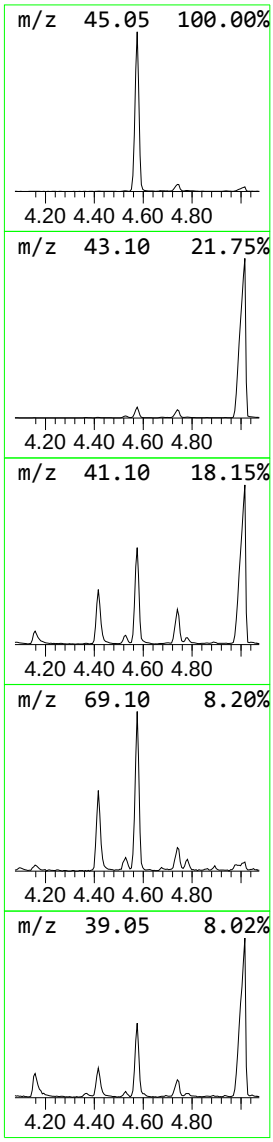
****

Peak Number 9 1-Butene, 4-methoxy Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	31.94 ng	1391340	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	50
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	39
4	4-Penten-2-ol	86	C5H10O	000625-31-0	38
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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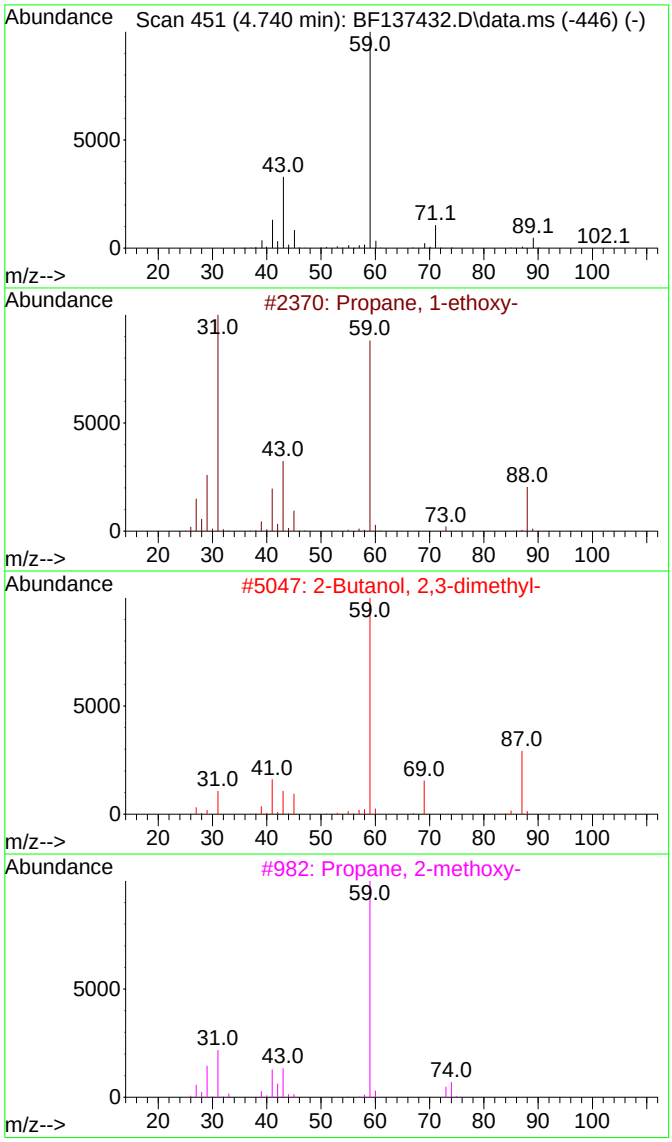
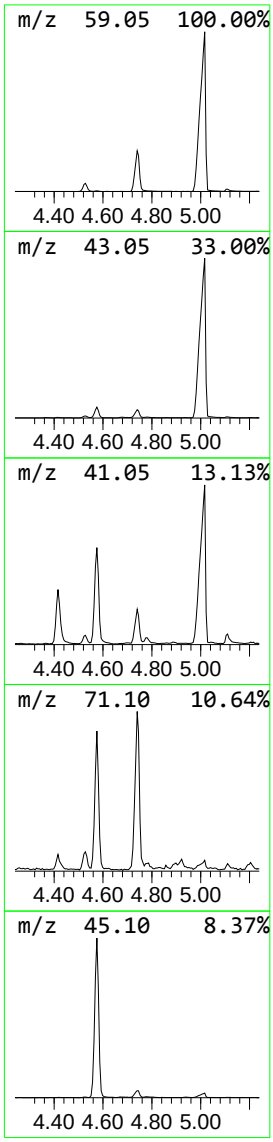
Peak Number 10 unknown4.740 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.740	16.29 ng	709363	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	38
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	38
3	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9
4	Butanoic acid, 2-hydroxy-, methy...	118	C5H10O3	029674-47-3	9
5	3-Pentanol	88	C5H12O	000584-02-1	9





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ClientSampleId :
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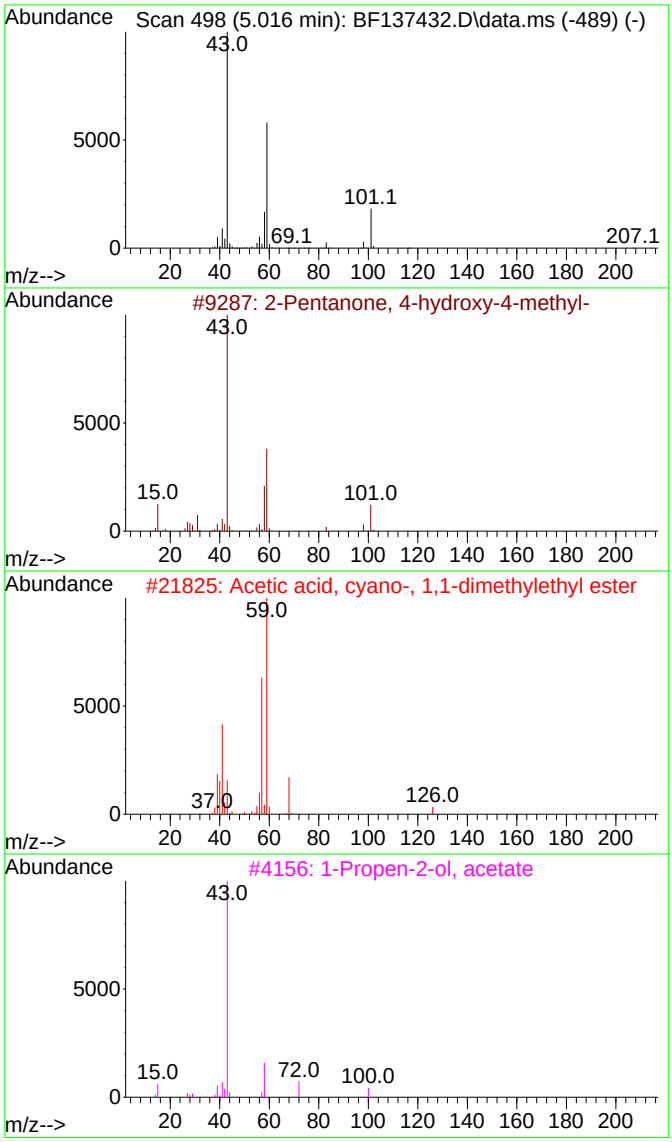
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

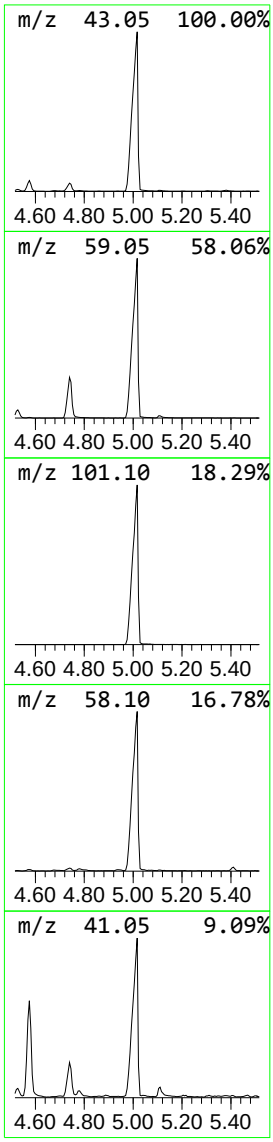
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	166.08 ng	7233590	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	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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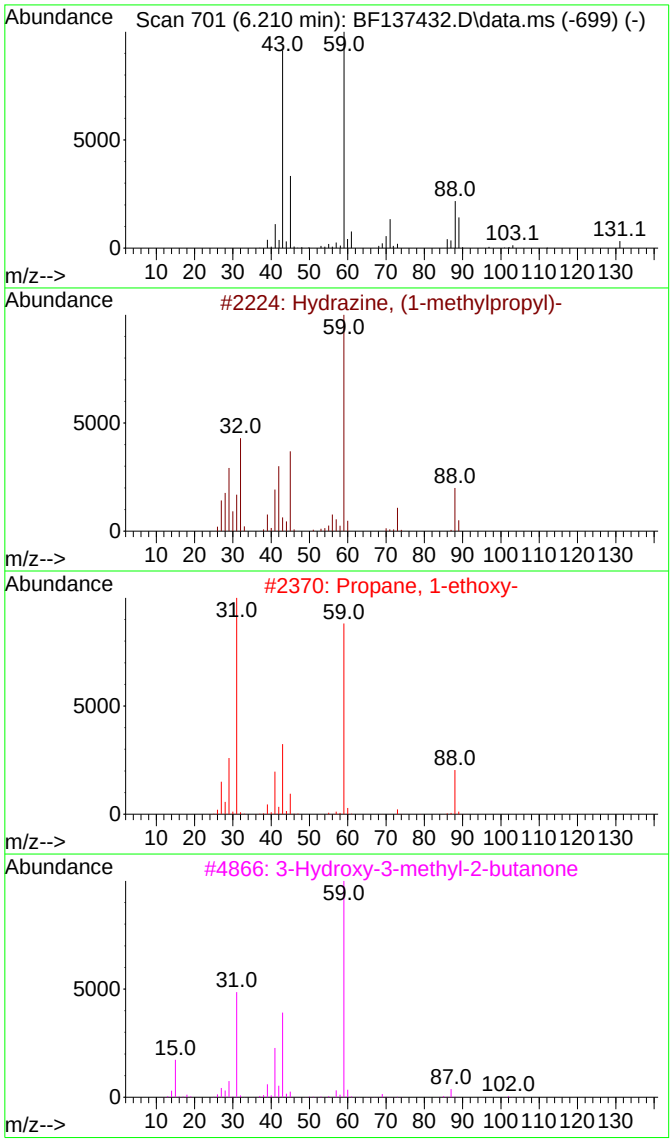
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

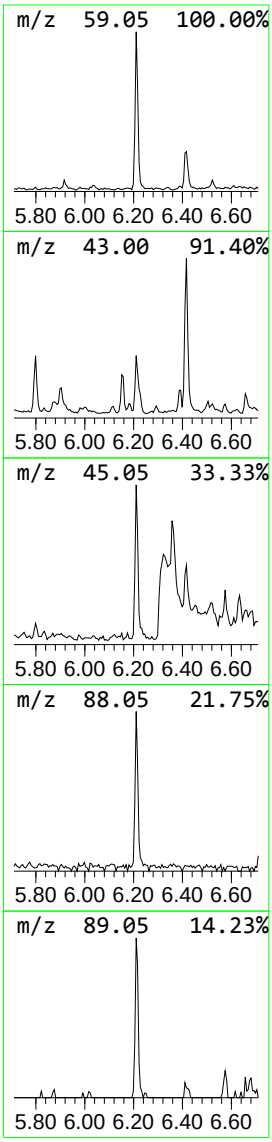
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Hydrazine, (1-methylpropyl)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.210	3.75 ng	163228	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, (1-methylpropyl)-	88	C4H12N2	030924-14-2	64
2	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	53
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	43
4	Tetraglyme	222	C10H22O5	000143-24-8	42
5	Butanamide	87	C4H9NO	000541-35-5	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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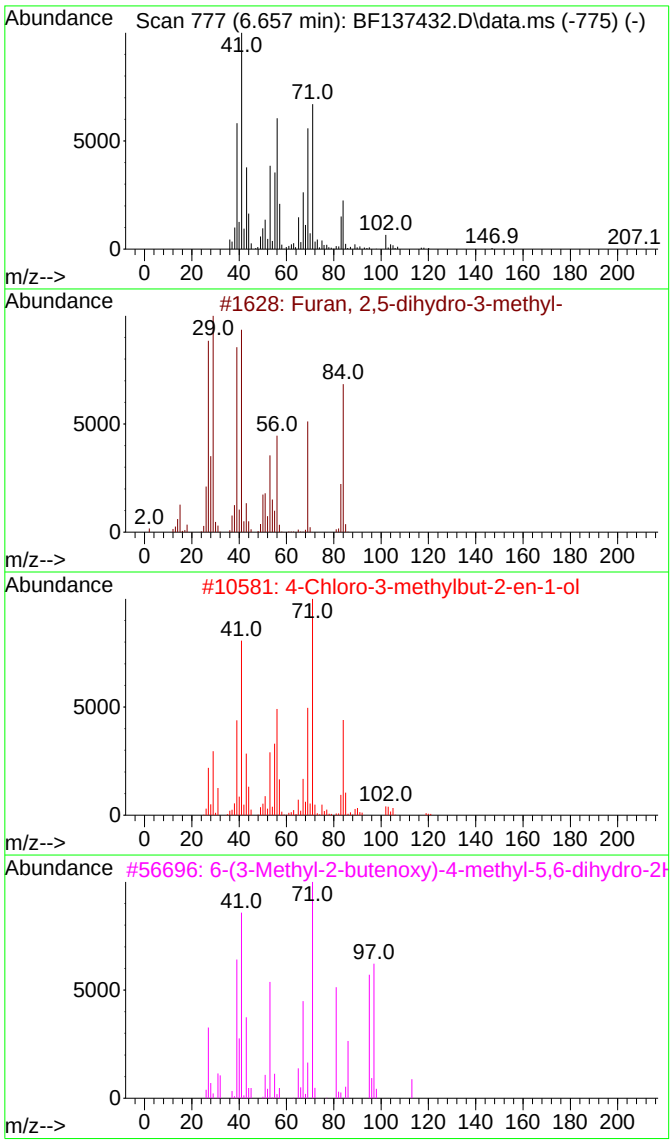
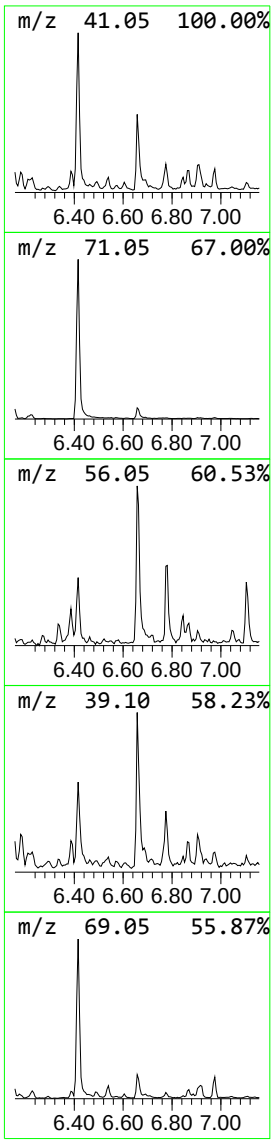
Peak Number 13 Furan, 2,5-dihydro-3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.657	5.61 ng	244483	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-3-methyl-	84	C5H8O	001708-31-2	72
2	4-Chloro-3-methylbut-2-en-1-ol	120	C5H9ClO	053170-97-1	59
3	6-(3-Methyl-2-butenoxy)-4-methyl...	182	C11H18O2	1000432-15-5	50
4	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	40
5	2-Methyl-2-vinyloxirane	84	C5H8O	001838-94-4	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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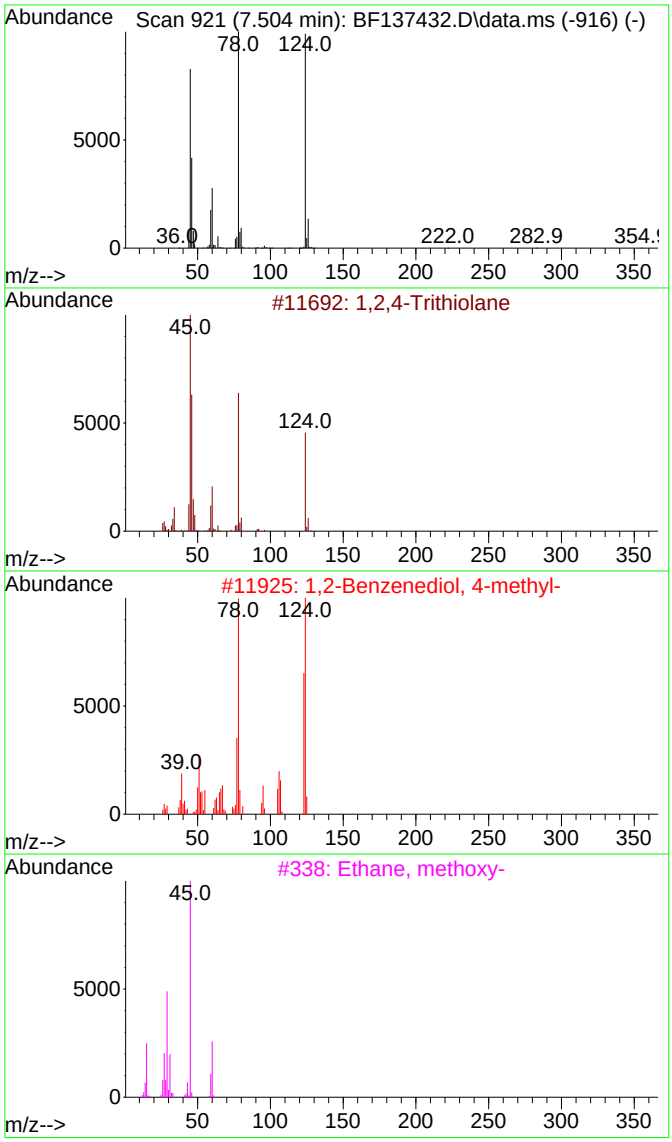
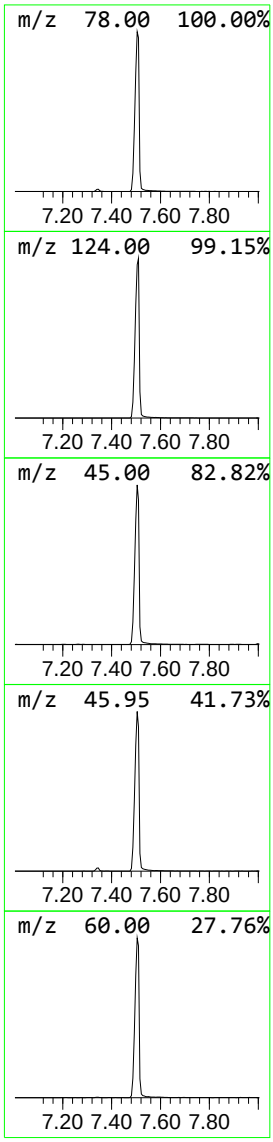
Peak Number 14 1,2,4-Trithiolane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.504	108.68 ng	6206000	Naphthalene-d8	8.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	91
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	42
3	Ethane, methoxy-	60	C3H8O	000540-67-0	9
4	Benzene	78	C6H6	000071-43-2	9
5	Fumaronitrile	78	C4H2N2	000764-42-1	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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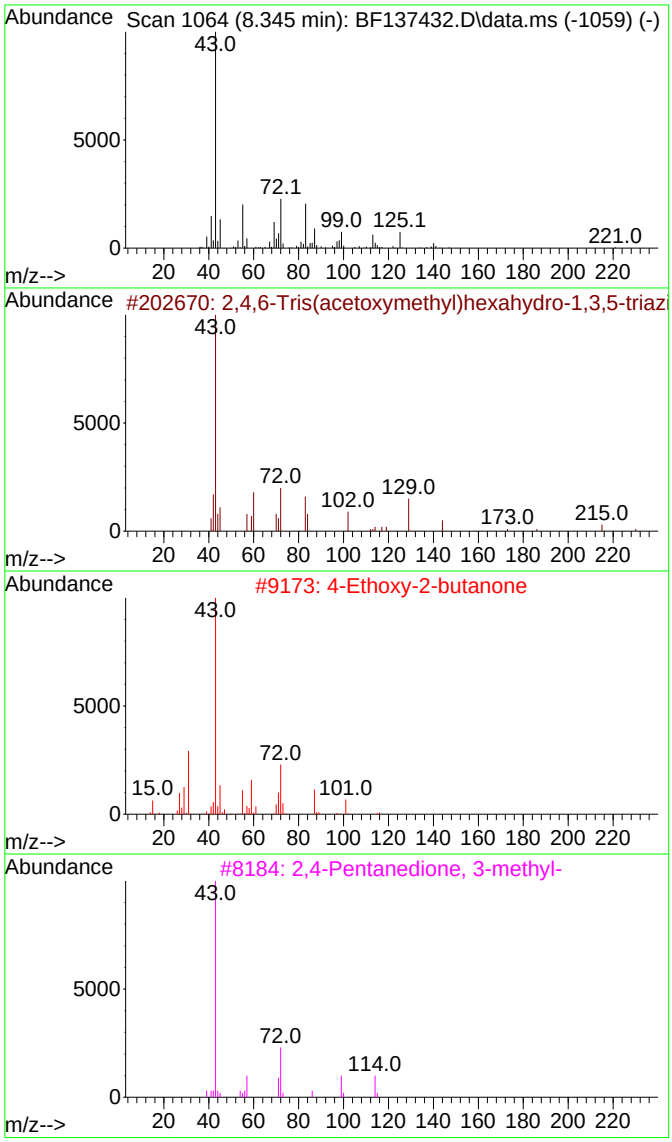
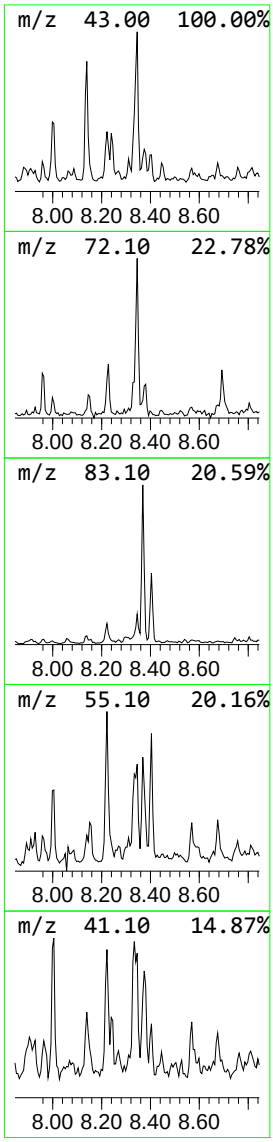
Peak Number 15 unknown8.345 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	3.83 ng	218849	Naphthalene-d8	8.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Tris(acetoxymethyl)hexahyd...	303	C12H21N3O6	1000090-49-5	25
2	4-Ethoxy-2-butanone	116	C6H12O2	060044-74-8	16
3	2,4-Pentanedione, 3-methyl-	114	C6H10O2	000815-57-6	14
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	11
5	5,6-Dihydro-4-methoxy-2H-pyran	114	C6H10O2	017327-22-9	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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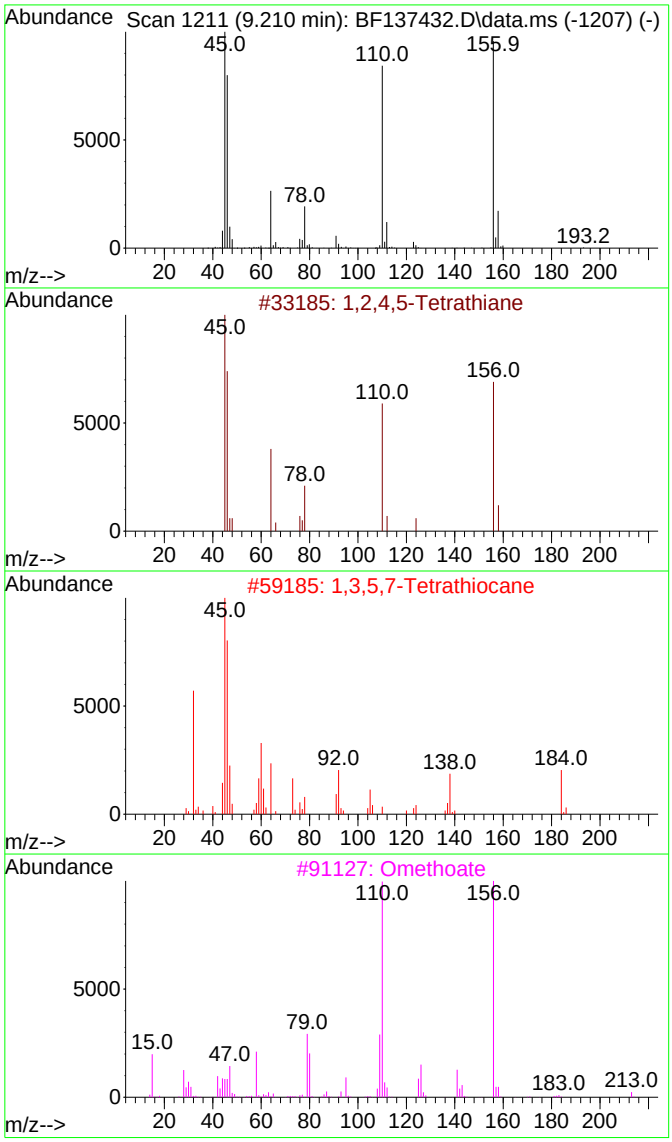
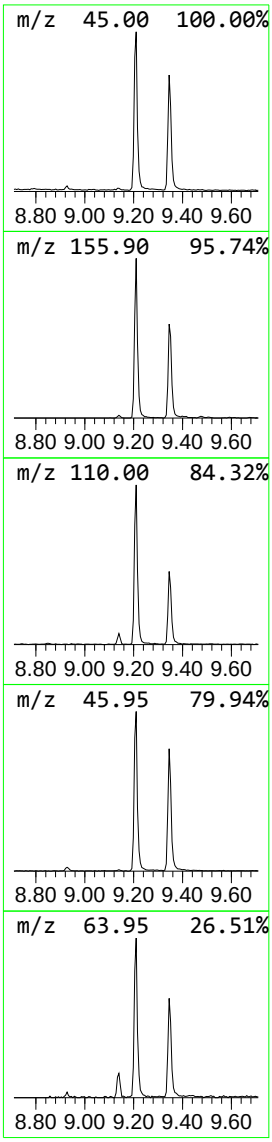
Peak Number 16 1,2,4,5-Tetrathiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	7.36 ng	537239	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	56
2	1,3,5,7-Tetrathiocane	184	C4H8S4	002373-00-4	17
3	Omethoate	213	C5H12NO4PS	001113-02-6	17
4	Tetrasulfur tetranitride	184	N4S4	1010443-95-7	10
5	2,3'-Dipyridyl	156	C10H8N2	000581-50-0	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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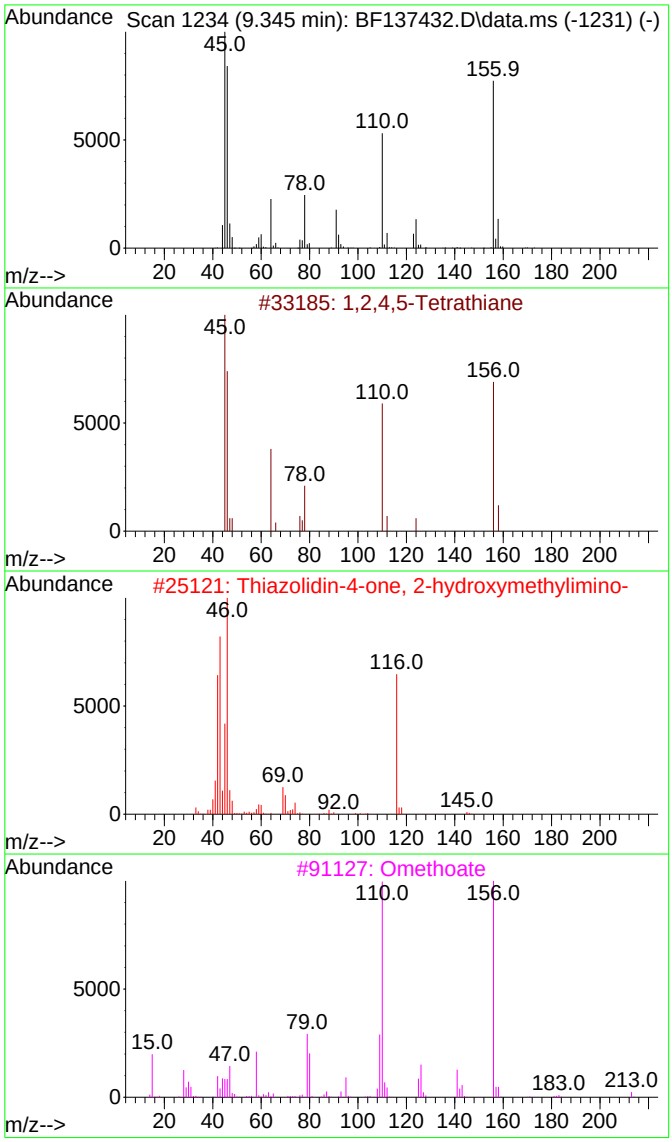
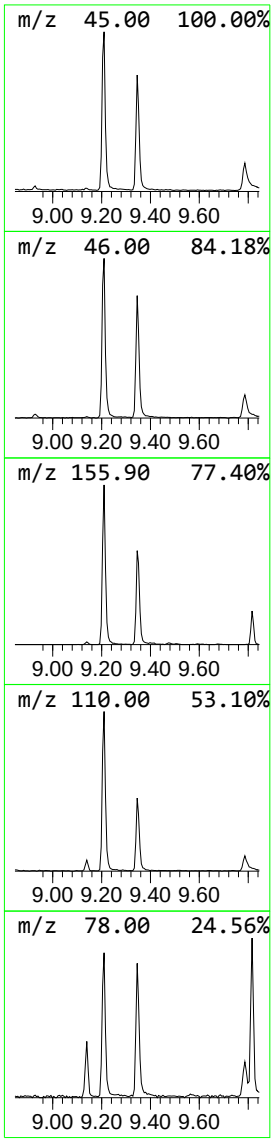
Peak Number 17 unknown9.345 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	5.46 ng	398068	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	86
2	Thiazolidin-4-one, 2-hydroxymeth...	146	C4H6N2O2S	104959-22-0	14
3	Omethoate	213	C5H12NO4PS	001113-02-6	12
4	[1,2,3,4]Tetrathiane	156	C2H4S4	000290-81-3	10
5	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	10





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TIC Library : C:\Database\NIST20.L
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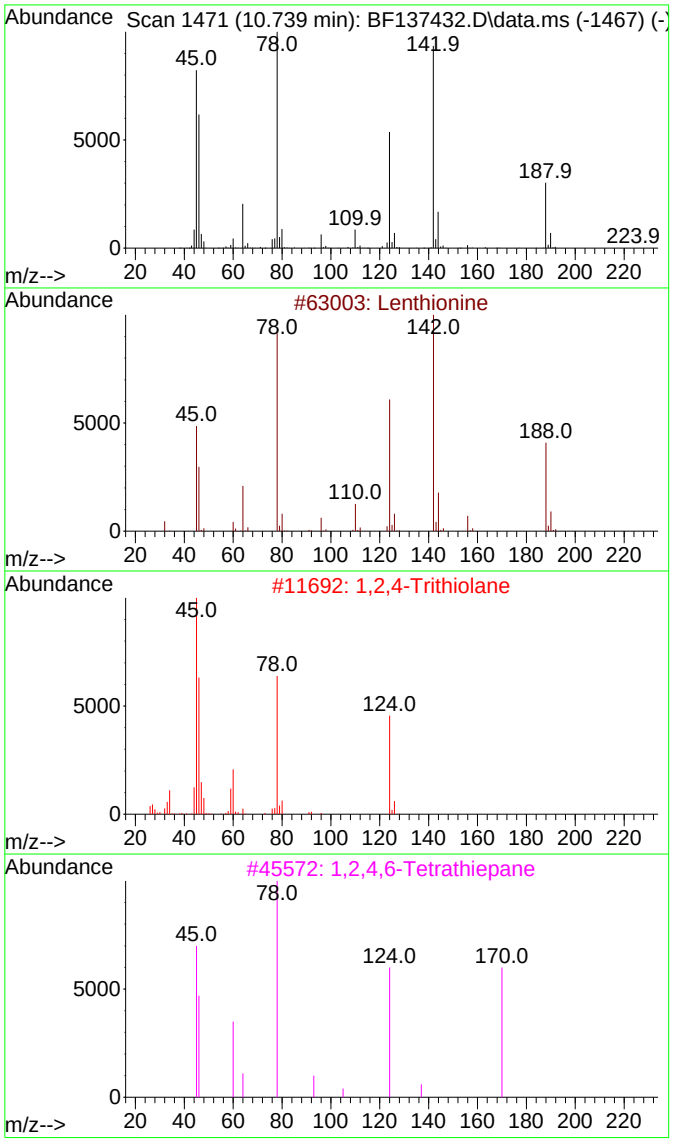
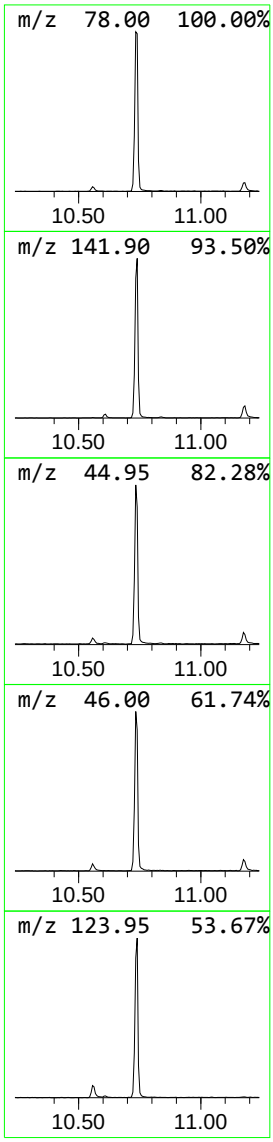
Peak Number 18 Lenthionine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	16.70 ng	1424650	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	59
2	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
3	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	50
4	4-Chloro-2-nitrobenzyl alcohol	187	C7H6ClNO3	022996-18-5	23
5	1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

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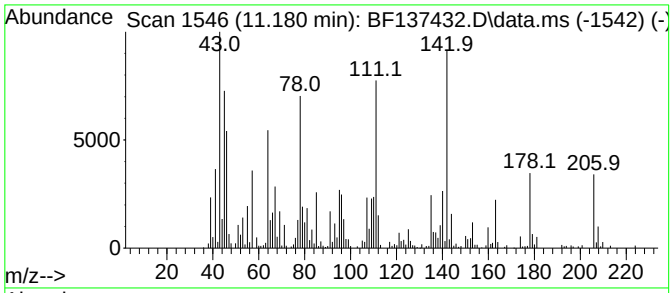
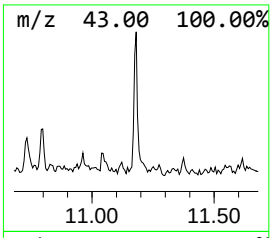
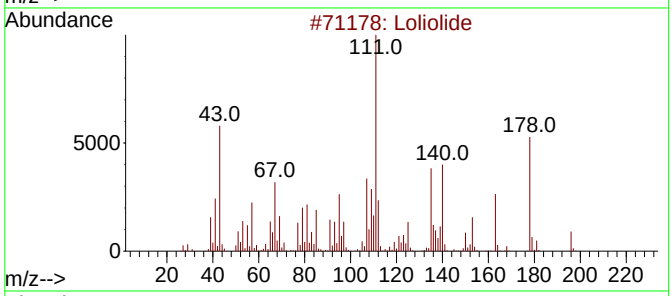
Peak Number 19 unknown11.181 Concentration Rank 17

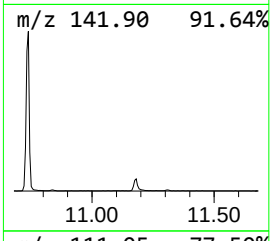
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	3.89 ng	331578	Phenanthrene-d10	11.310

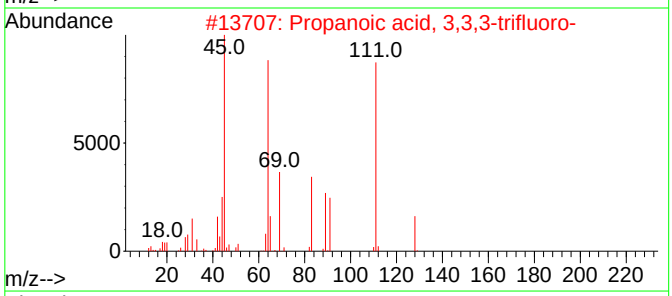
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Loliolide	196	C11H16O3	005989-02-6	38
2	Propanoic acid, 3,3,3-trifluoro-	128	C3H3F3O2	002516-99-6	32
3	2-Fluoro-6-methylpyridine	111	C6H6FN	000407-22-7	32
4	Acetone-D6	64	C3D6O	000666-52-4	27
5	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	27

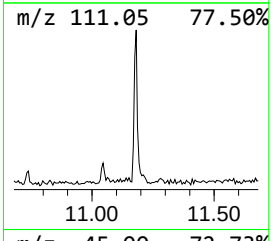


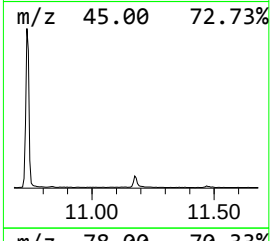


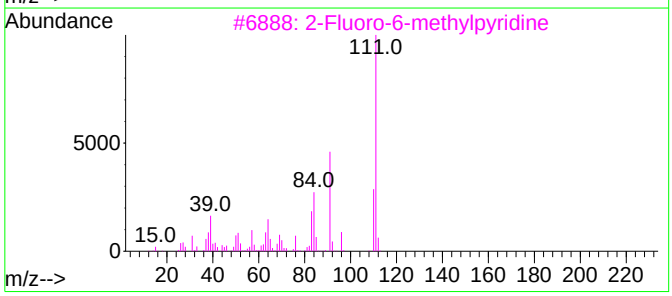


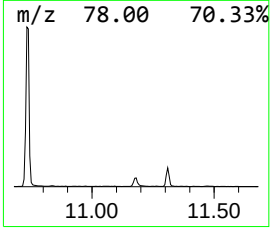












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

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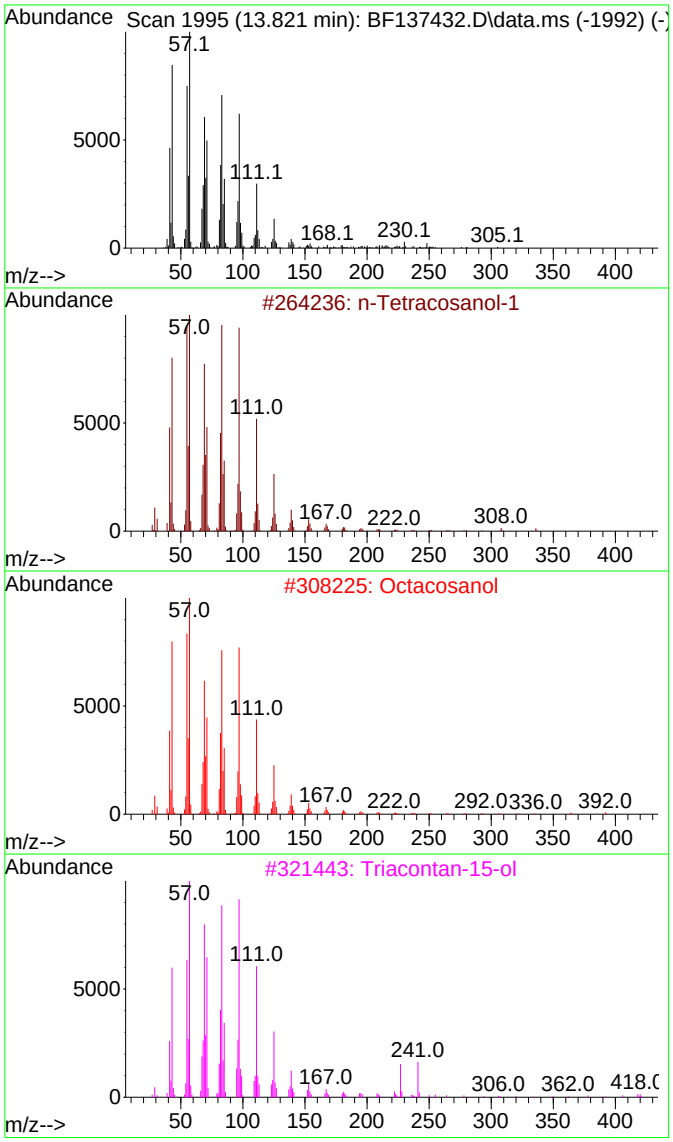
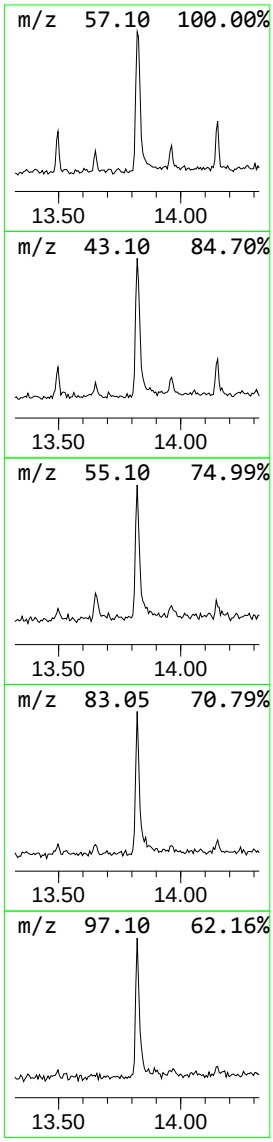
Peak Number 20 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	5.99 ng	462718	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Triacontan-15-ol	438	C30H62O	031849-26-0	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137432.D
Acq On : 28 Feb 2024 19:50
Operator : CG\JU
Sample : P1523-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-ol	2.134	165.3	ng	7199520	1	6.781	871102	20.0
unknown3.587	3.587	7.1	ng	309039	1	6.781	871102	20.0
3-Methyl-3-chlo...	3.881	5.4	ng	237010	1	6.781	871102	20.0
2-Buten-1-ol, 2...	3.957	5.4	ng	235971	1	6.781	871102	20.0
unknown3.981	3.981	6.8	ng	295812	1	6.781	871102	20.0
2-Butenal, 3-me...	4.157	4.9	ng	212516	1	6.781	871102	20.0
unknown4.416	4.416	7.8	ng	338076	1	6.781	871102	20.0
Propanoic acid,...	4.528	3.6	ng	156485	1	6.781	871102	20.0
1-Butene, 4-met...	4.575	31.9	ng	1391340	1	6.781	871102	20.0
unknown4.740	4.740	16.3	ng	709363	1	6.781	871102	20.0
2-Pentanone, 4-...	5.016	166.1	ng	7233590	1	6.781	871102	20.0
Hydrazine, (1-m...	6.210	3.8	ng	163228	1	6.781	871102	20.0
Furan, 2,5-dihy...	6.657	5.6	ng	244483	1	6.781	871102	20.0
1,2,4-Trithiolane	7.504	108.7	ng	6206000	2	8.057	1142050	20.0
unknown8.345	8.345	3.8	ng	218849	2	8.057	1142050	20.0
1,2,4,5-Tetrath...	9.210	7.4	ng	537239	3	9.816	1459160	20.0
unknown9.345	9.345	5.5	ng	398068	3	9.816	1459160	20.0
Lenthionine	10.739	16.7	ng	1424650	4	11.310	1706410	20.0
unknown11.181	11.181	3.9	ng	331578	4	11.310	1706410	20.0
n-Tetracosanol-1	13.822	6.0	ng	462718	5	13.969	1544020	20.0