LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	3	8	23	rVB	2604463	3065860	59.77%	10.223%
2	3.746	107	112	118	rBV2	43088	71867	1.40%	0.240%
3	4.069	161	167	174	rBV	186925	304141	5.93%	1.014%
4	4.246	191	197	204	rBV	62445	92110	1.80%	0.307%
5	4.458	228	233	244	rVB	69528	103099	2.01%	0.344%
6	4.640	259	264	269	rVV	270780	396425	7.73%	1.322%
7	4.693	269	273	285	rVB	176091	260691	5.08%	0.869%
8	5.022	322	329	338	rBV	1679498	2429372	47.36%	8.101%
9	5.469	399	405	413	rBV	382247	624182	12.17%	2.081%
10	5.793	455	460	466	rBV3	36392	59272	1.16%	0.198%
11	7.069	670	677	684	rBV	654793	1063687	20.74%	3.547%
12	7.593	760	766	774	rBV2	53402	100229	1.95%	0.334%
13	7.899	812	818	824	rVB	235174	375361	7.32%	1.252%
14	8.140	852	859	864	rBV2	36918	68773	1.34%	0.229%
15	8.869	978	983	988	rBV2	38616	85790	1.67%	0.286%
16	9.069	1010	1017	1028	rVB	660720	1136517	22.16%	3.790%
17	9.357	1057	1066	1070	rBV7	23365	64717	1.26%	0.216%
18	9.434	1071	1079	1088	rVV	1886607	3520020	68.62%	11.737%
19	9.975	1162	1171	1179	rBV6	28684	115989	2.26%	0.387%
20	10.057	1180	1185	1196	rVB4	31591	87860	1.71%	0.293%
21	10.698	1286	1294	1310	rVB	295964	543380	10.59%	1.812%
22	10.887	1320	1326	1340	rBV3	21476	60623	1.18%	0.202%
23	11.087	1350	1360	1366	rBV7	35936	107231	2.09%	0.358%
24	11.451	1415	1422	1428	rVV3	39408	79932	1.56%	0.267%
25	13.157	1705	1712	1729	rBV	1827152	2736253	53.34%	9.124%
26	13.298	1729	1736	1744	rVV	136823	226580	4.42%	0.756%
27	13.587	1778	1785	1793	rBV	109225	190259	3.71%	0.634%
28	14.457	1921	1933	1940	rBV2	71800	188968	3.68%	0.630%
29	14.534	1940	1946	1954	rVB	481962	782851	15.26%	2.610%
30	15.145	2042	2050	2055	rBV	55891	117652	2.29%	0.392%
31	16.028	2194	2200	2217	rVB	335435	554417	10.81%	1.849%
32	16.263	2234	2240	2252	rVB	426115	704728	13.74%	2.350%
33	17.063	2370	2376	2390	rVB2	118041	220491	4.30%	0.735%
34	17.292	2408	2415	2421	rBV	665635	1047241	20.42%	3.492%
35	18.186	2562	2567	2571	rBV	72119	115871	2.26%	0.386%
36	19.304	2753	2757	2762	rVB	52490	66616	1.30%	0.222%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.422	2773	2777	2781	rBV5	39326	67335	1.31%	0.225%
38	19.651	2813	2816	2819	rBV	45688	51938	1.01%	0.173%
39	19.857	2845	2851	2862	rBV	4316490	5129686	100.00%	17.105%
40	20.863	3019	3022	3027	rBV	77162	79729	1.55%	0.266%
41	21.104	3059	3063	3071	rVB	268080	324097	6.32%	1.081%
42	21.380	3105	3110	3115	rBV	903059	1313781	25.61%	4.381%
43	23.798	3515	3521	3530	rVB	581462	1254317	24.45%	4.182%

Sum of corrected areas: 29989938

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
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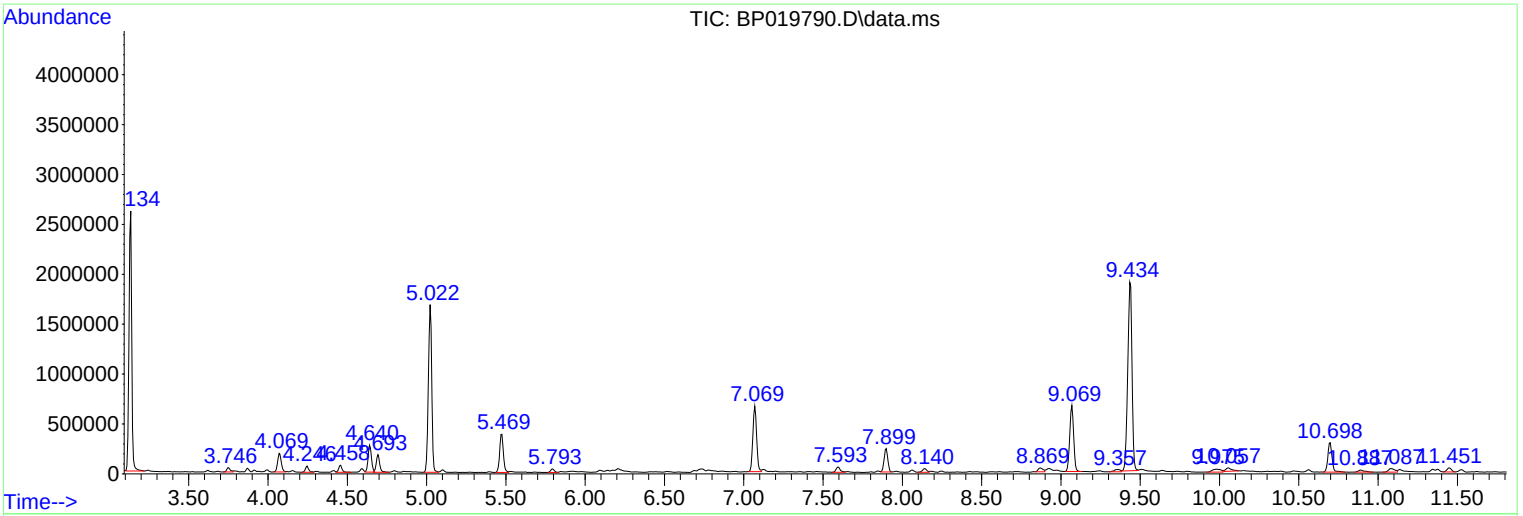
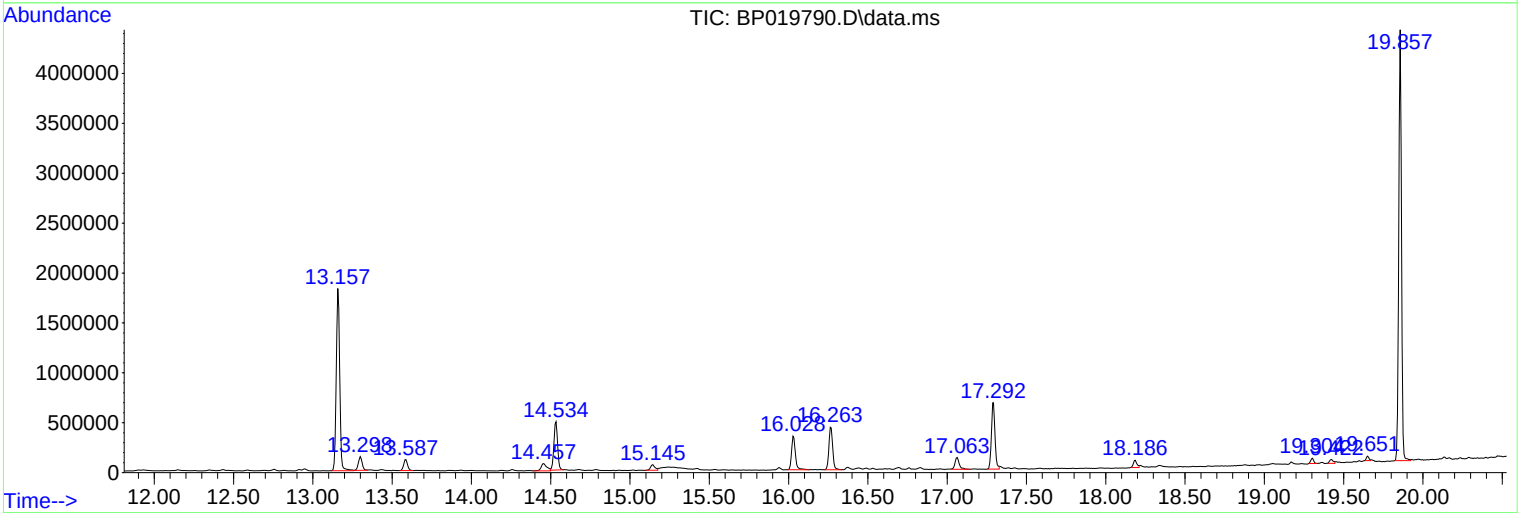
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

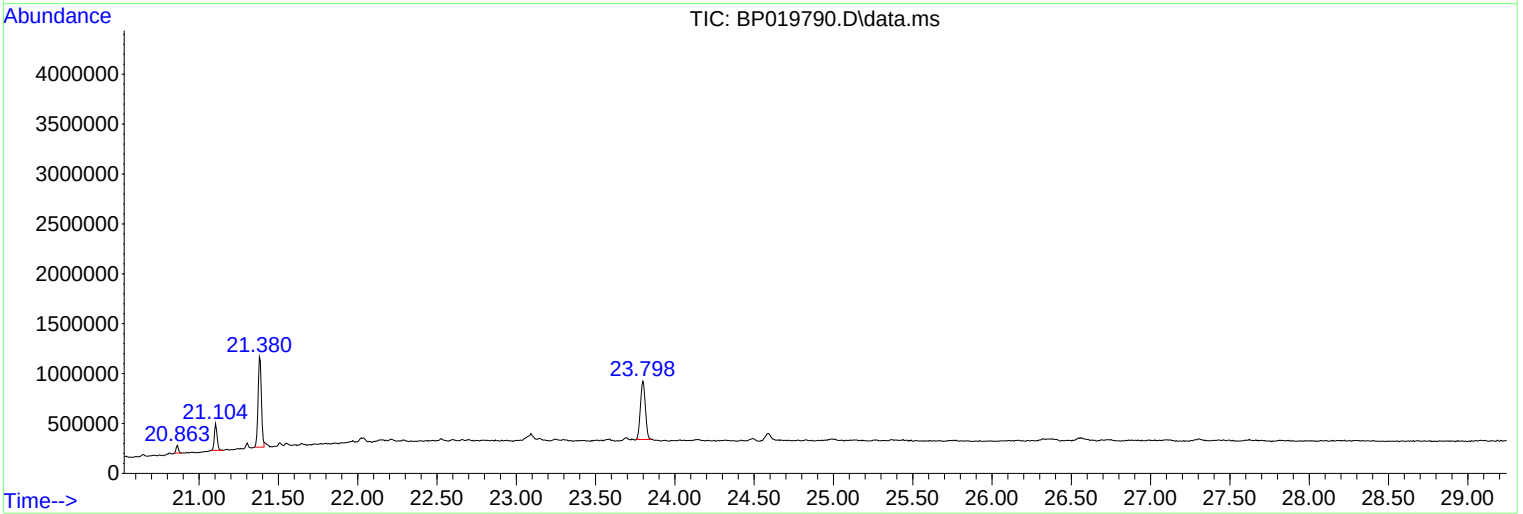
Instrument :
BNA_P
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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_P\Data\BP022024\
Data File : BP019790.D
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Operator : MA/JU
Sample : P1523-08
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

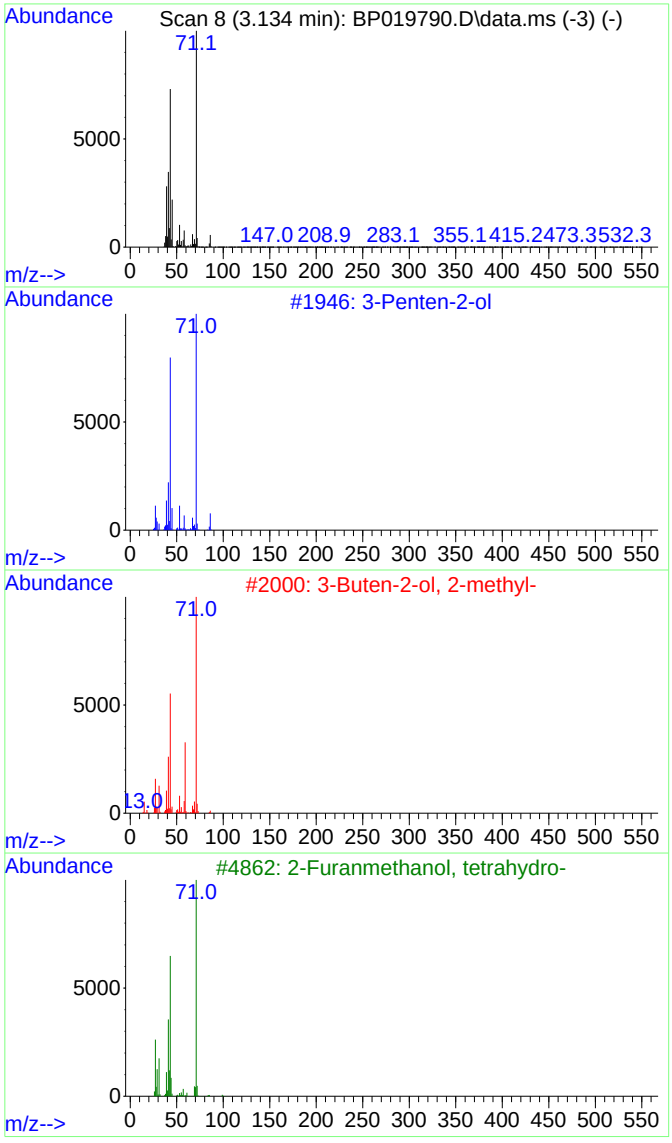
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

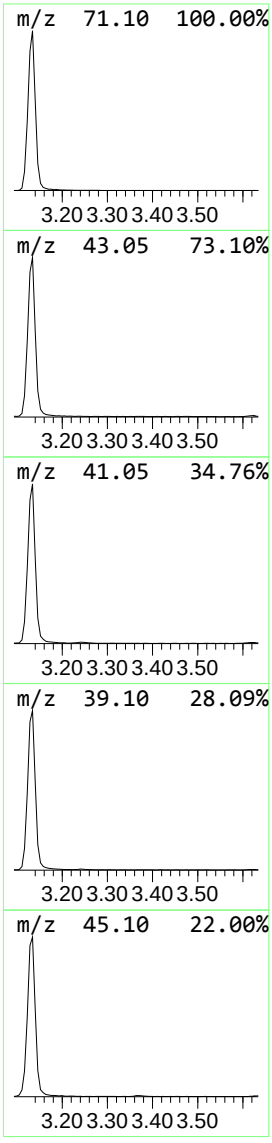
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	163.35 ng	3065860	1,4-Dichlorobenzene-d4	7.899

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	59
3	2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	50
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	45
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

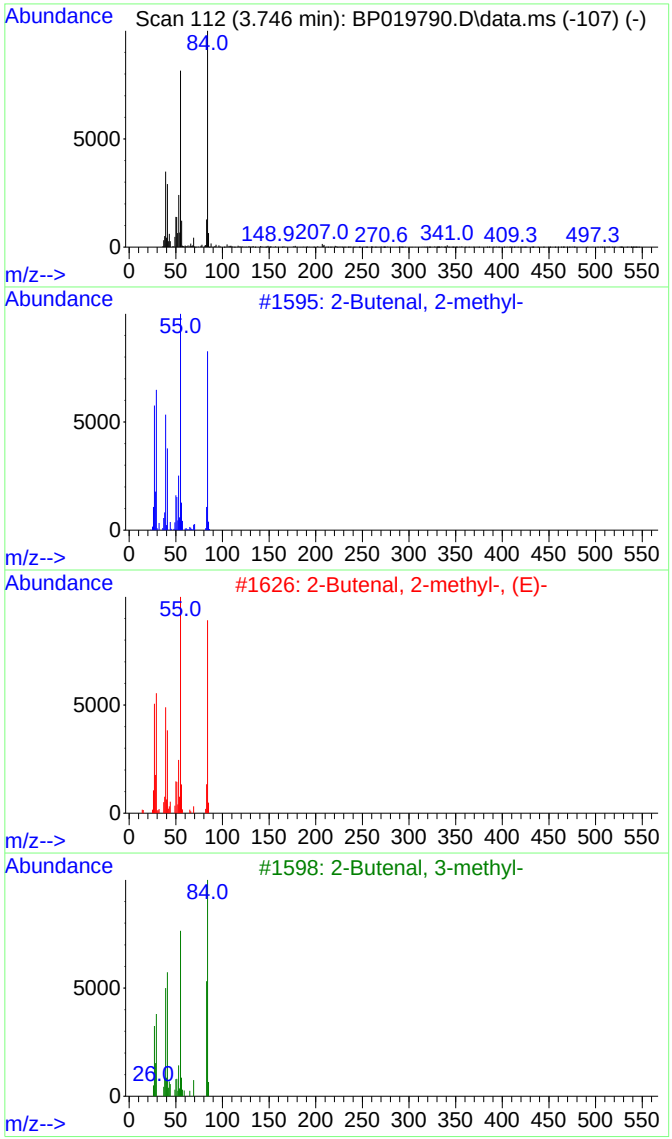
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

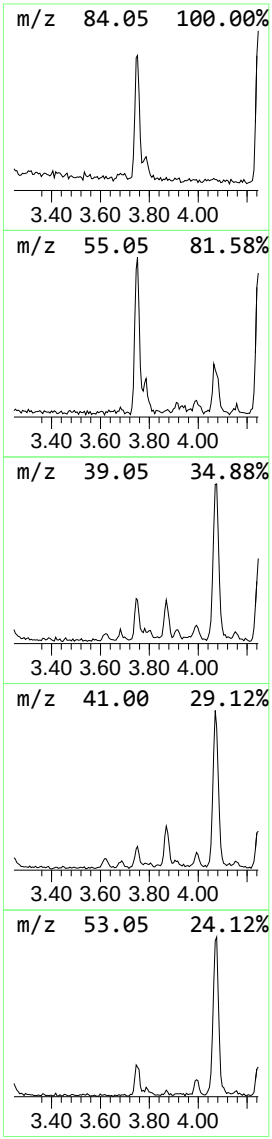
****

Peak Number 2 2-Butenal, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.746	3.83 ng	71867	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	91
2	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	91
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	87
4	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	45
5	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

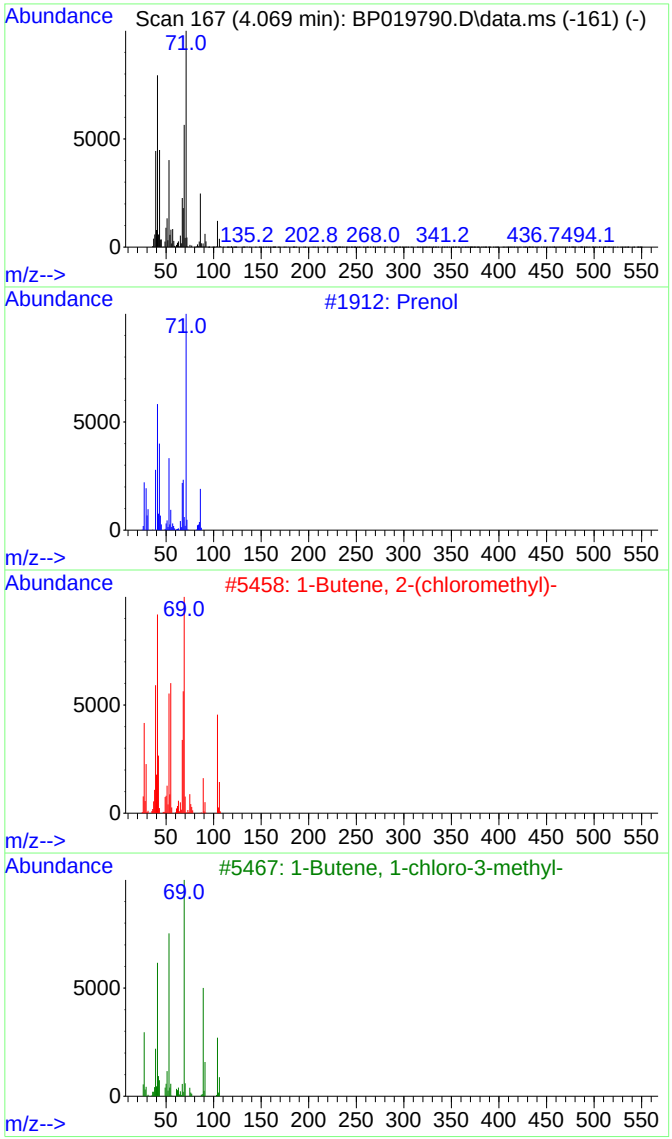
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

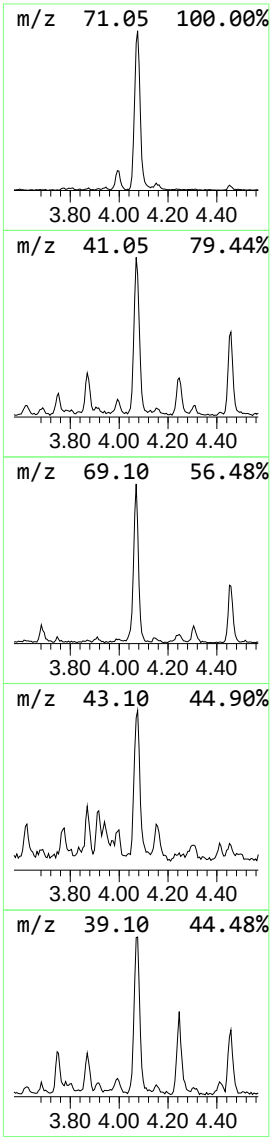
****

Peak Number 3 Prenol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.069	16.21 ng	304141	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	72
2	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	50
3	1-Butene, 1-chloro-3-methyl-	104	C5H9Cl	023010-00-6	43
4	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	43
5	2-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-65-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

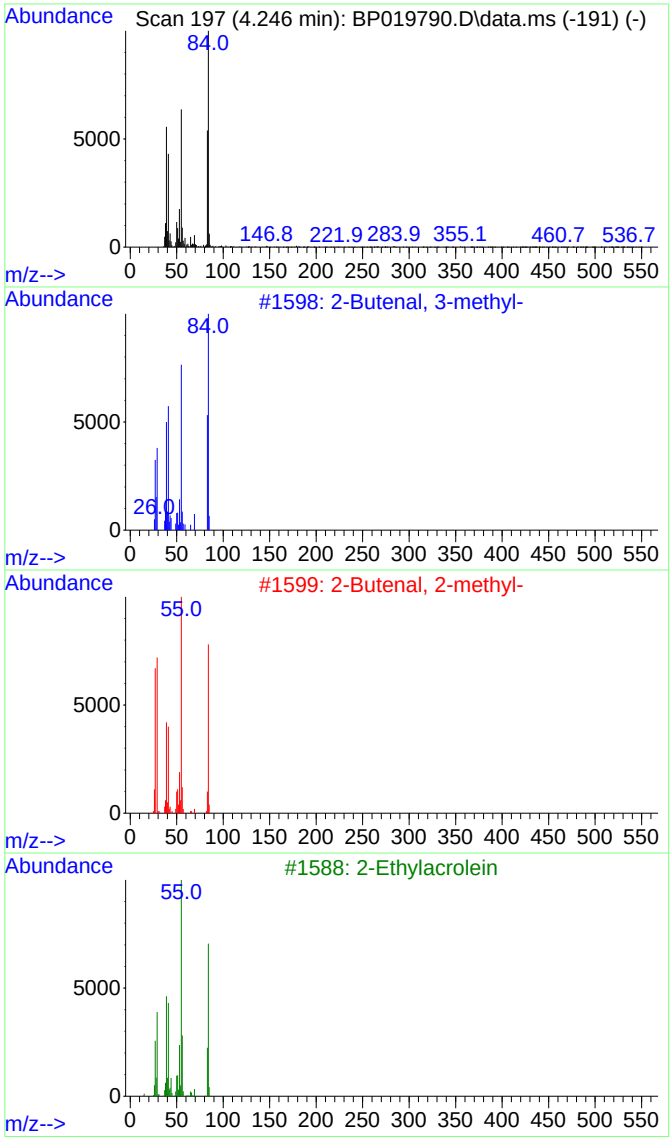
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

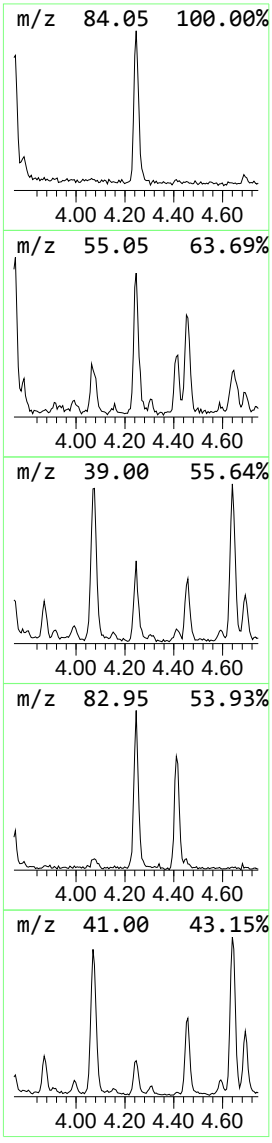
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butenal, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.246	4.91 ng	92110	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	81
2	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	50
3	2-Ethylacrolein	84	C5H8O	000922-63-4	50
4	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	50
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
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Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

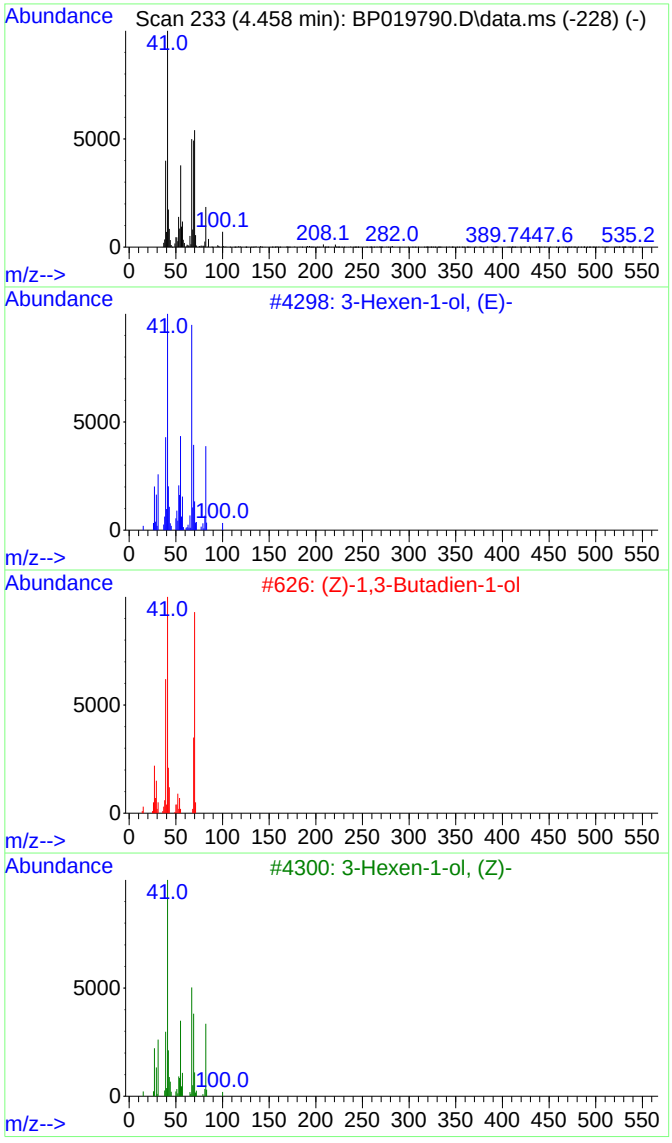
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

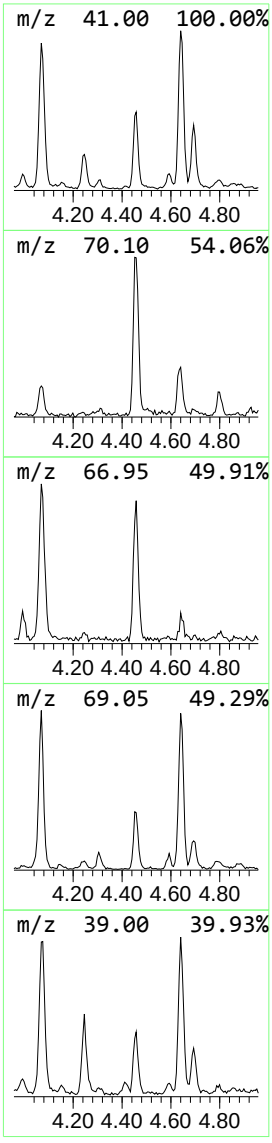
****

Peak Number 5 unknown4.458 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.458	5.49 ng	103099	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-1-ol, (E)-	100	C6H12O	000928-97-2	47
2	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	43
3	3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	43
4	2-Butenenitrile	67	C4H5N	004786-20-3	38
5	3-Hexen-1-ol	100	C6H12O	000544-12-7	35





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Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

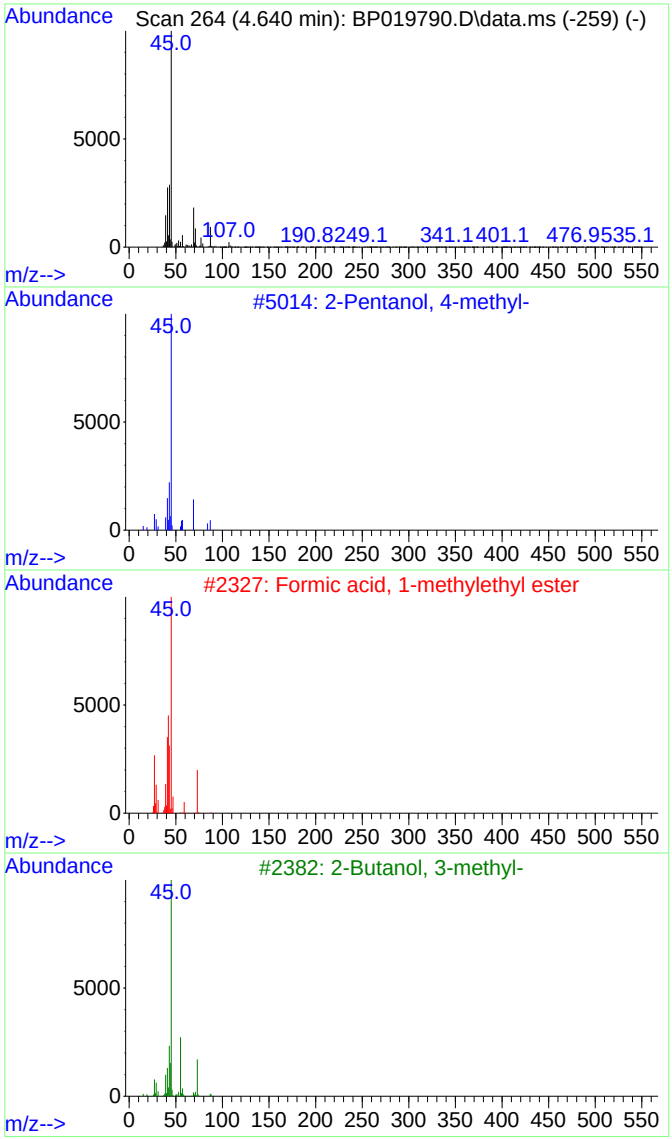
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

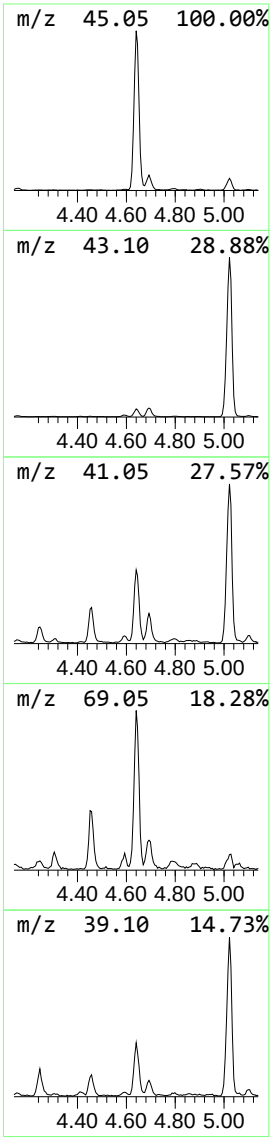
****

Peak Number 6 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	21.12 ng	396425	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	50
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	42
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	40
5	2-Hexanol	102	C6H14O	000626-93-7	40





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Data File : BP019790.D
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Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

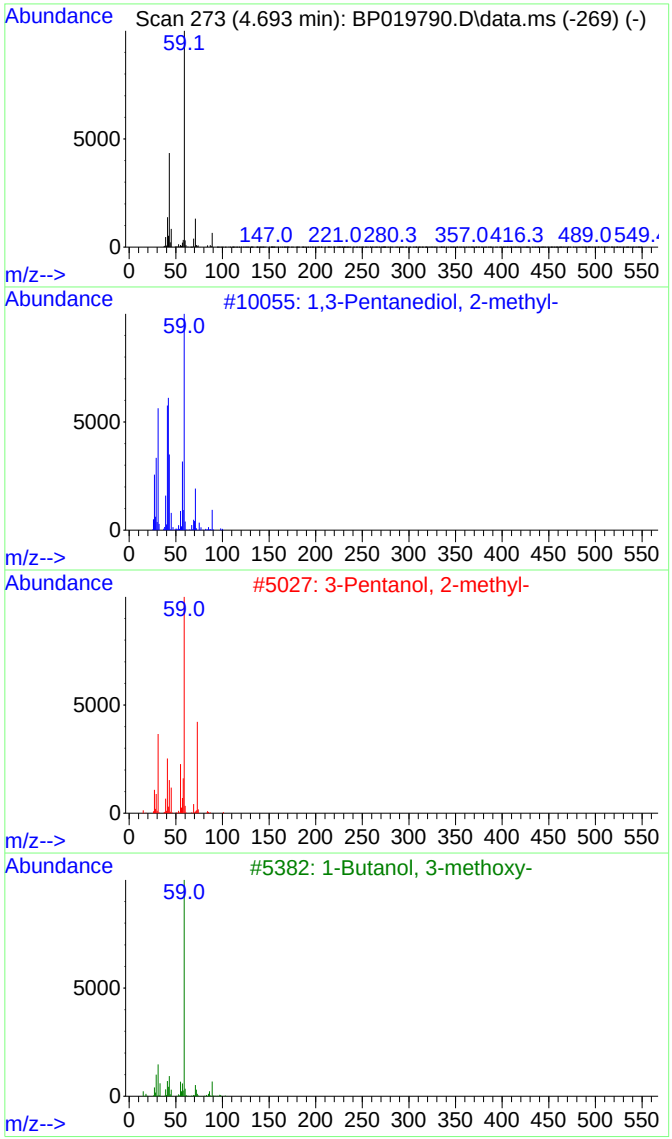
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

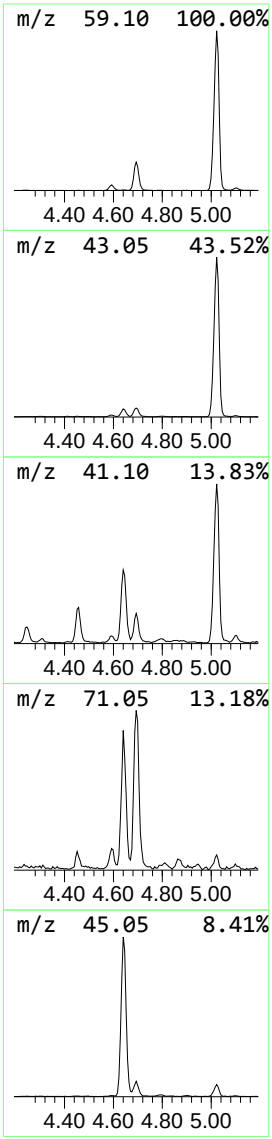
****

Peak Number 7 unknown4.693 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.693	13.89 ng	260691	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2-methyl-	118	C6H14O2	000149-31-5	39
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	36
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

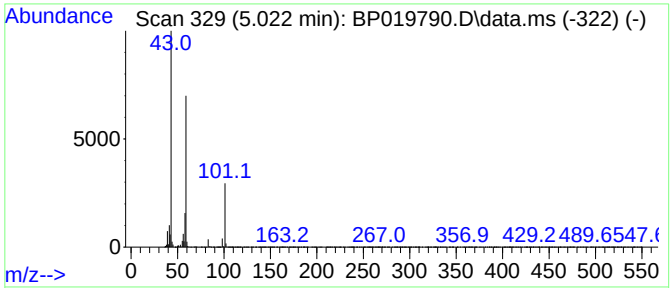
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

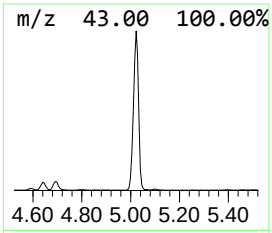
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

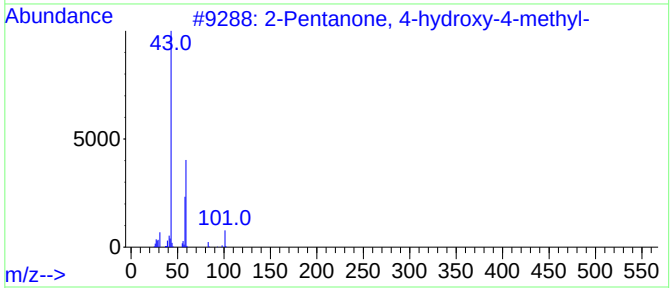
****
Peak Number 8 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

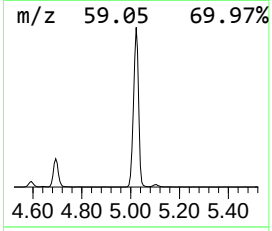
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	129.44 ng	2429370	1,4-Dichlorobenzene-d4	7.899

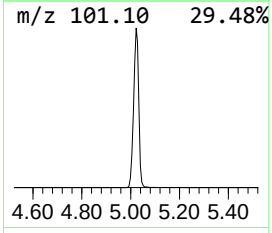
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

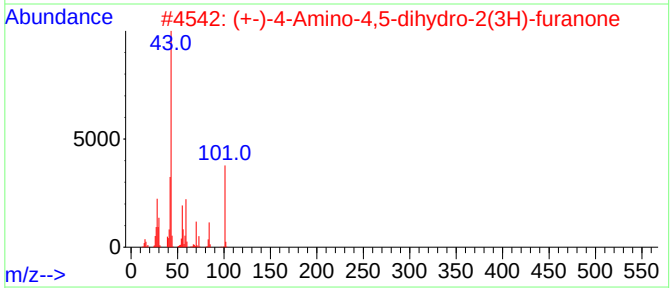


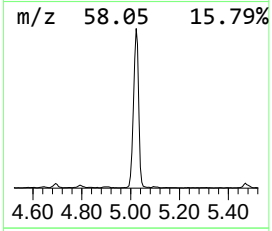


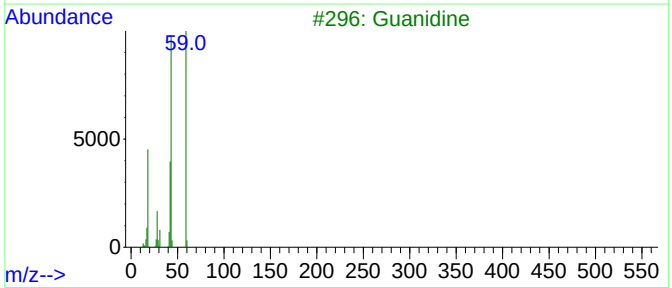


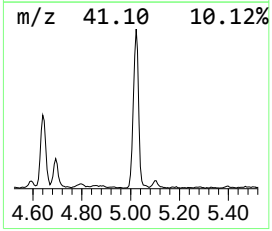












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Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

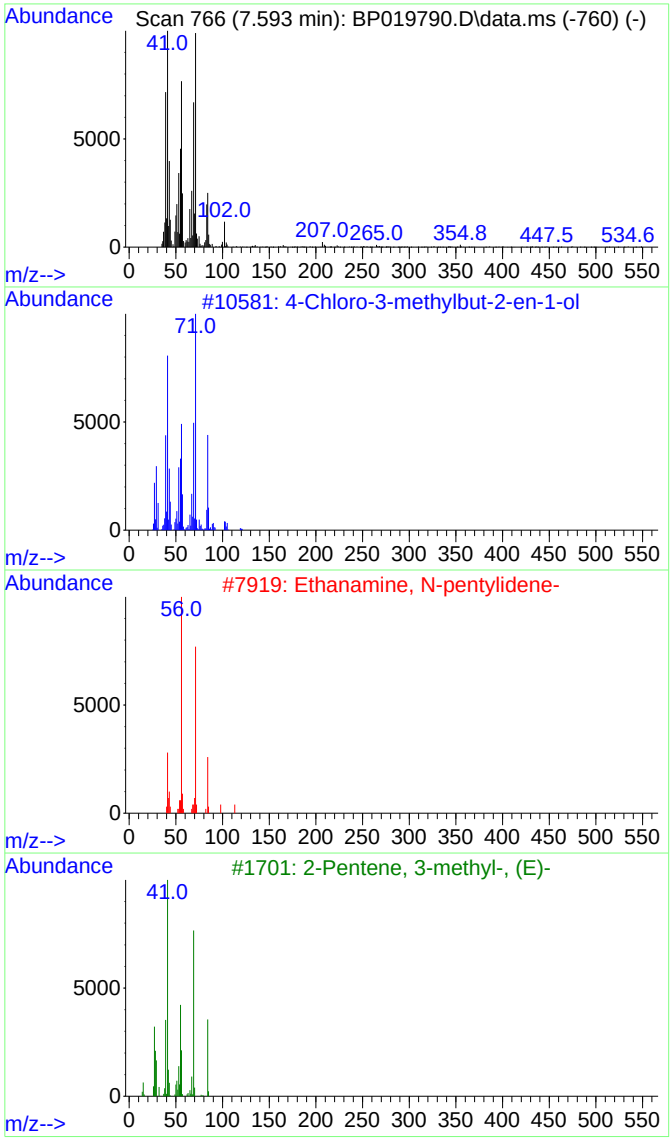
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

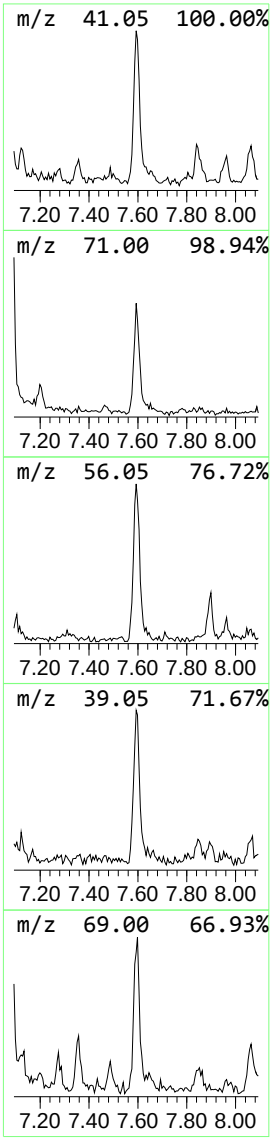
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Chloro-3-methylbut-2-en-1-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.593	5.34 ng	100229	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-3-methylbut-2-en-1-ol	120	C5H9ClO	053170-97-1	59
2	Ethanamine, N-pentylidene-	113	C7H15N	010599-76-5	50
3	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	43
4	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	43
5	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	35





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Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

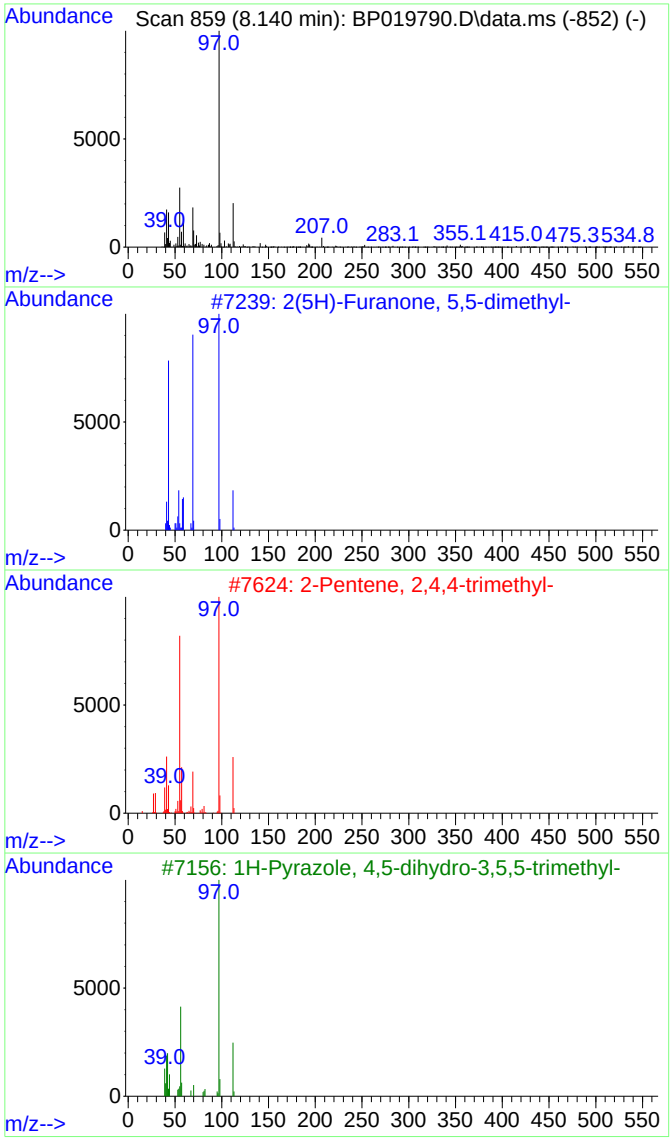
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

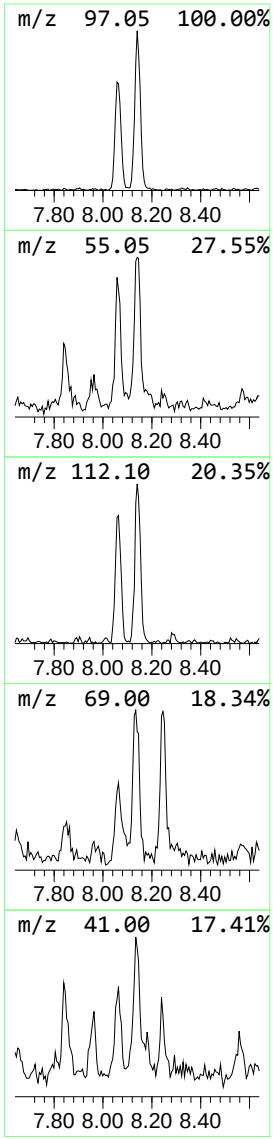
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2(5H)-Furanone, 5,5-dimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	3.66 ng	68773	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	72
2	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	64
3	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	64
4	1H-Pyrazole, 4,5-dihydro-3,4,5-t...	112	C6H12N2	022591-95-3	59
5	2-Pentene, 3,4,4-trimethyl-	112	C8H16	000598-96-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
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Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

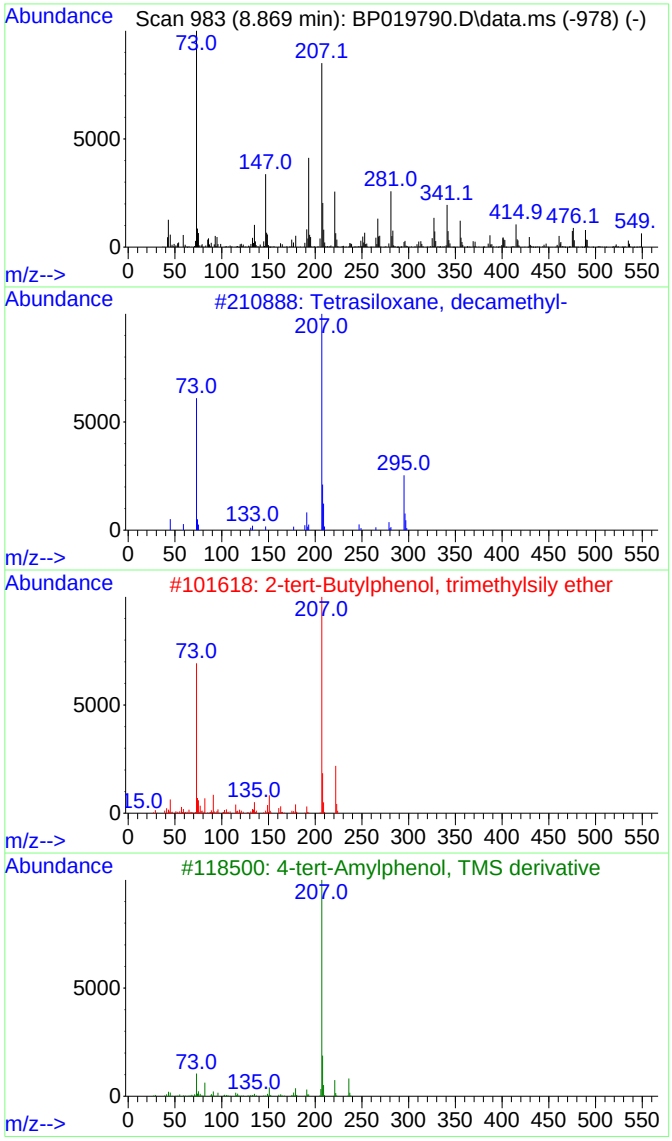
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

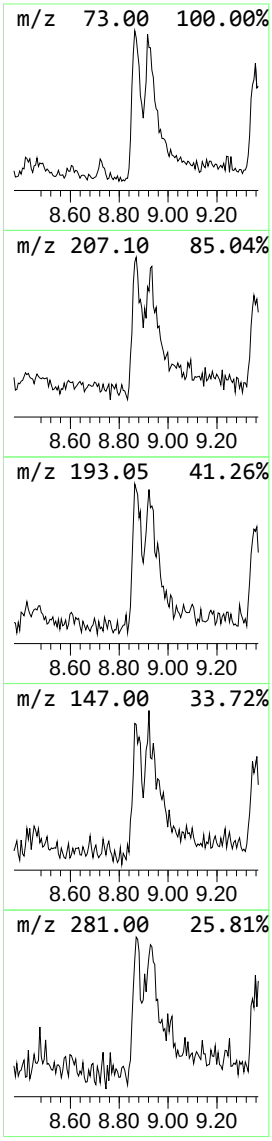
****

Peak Number 11 unknown8.869 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	4.57 ng	85790	1,4-Dichlorobenzene-d4	7.899

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	43
2	2-tert-Butylphenol, trimethylsil...	222	C13H22OSi	025282-58-0	38
3	4-tert-Amylphenol, TMS derivative	236	C14H24OSi	1000373-05-7	38
4	7,7,9,9,11,11-Hexamethyl-3,6,8,1...	384	C14H36O6Si3	1000375-89-1	38
5	Tetrahydrorhombifoline	248	C15H24N2O	003382-84-1	35





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

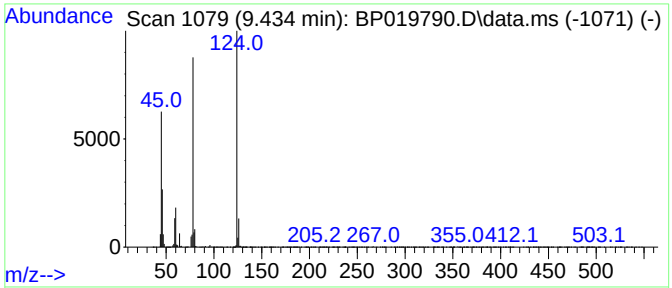
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

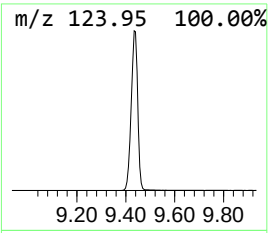
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

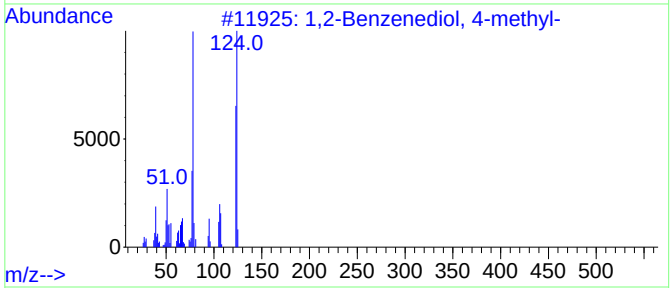
****
Peak Number 12 1,2-Benzenediol, 4-methyl- Concentration Rank 2

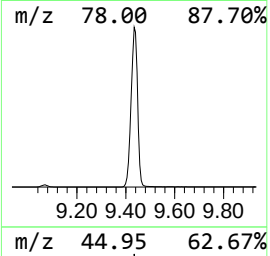
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.434	129.56 ng	3520020	Naphthalene-d8	10.698

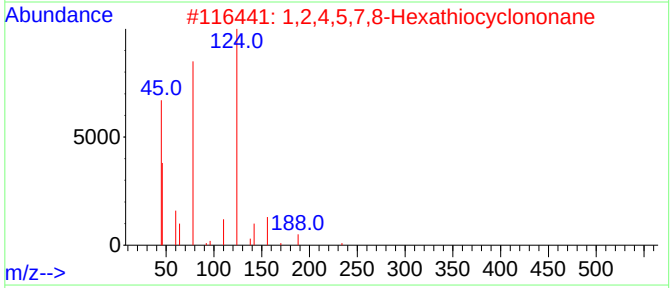
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	Benzene	78	C6H6	000071-43-2	9
5	Dipyrithione	252	C10H8N2O2S2	003696-28-4	9

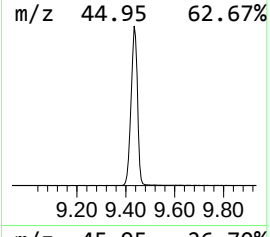


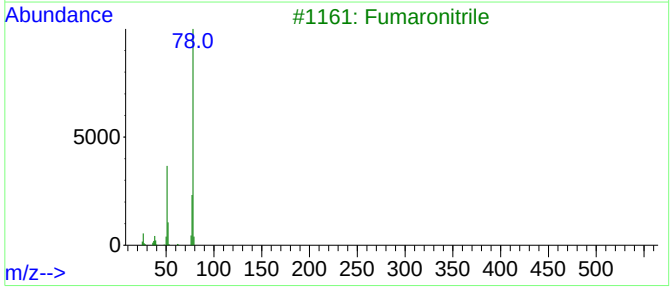


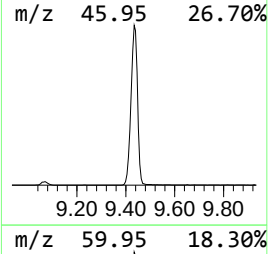


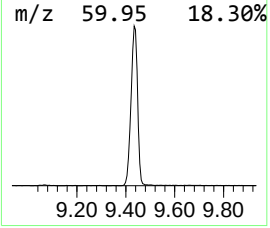












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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

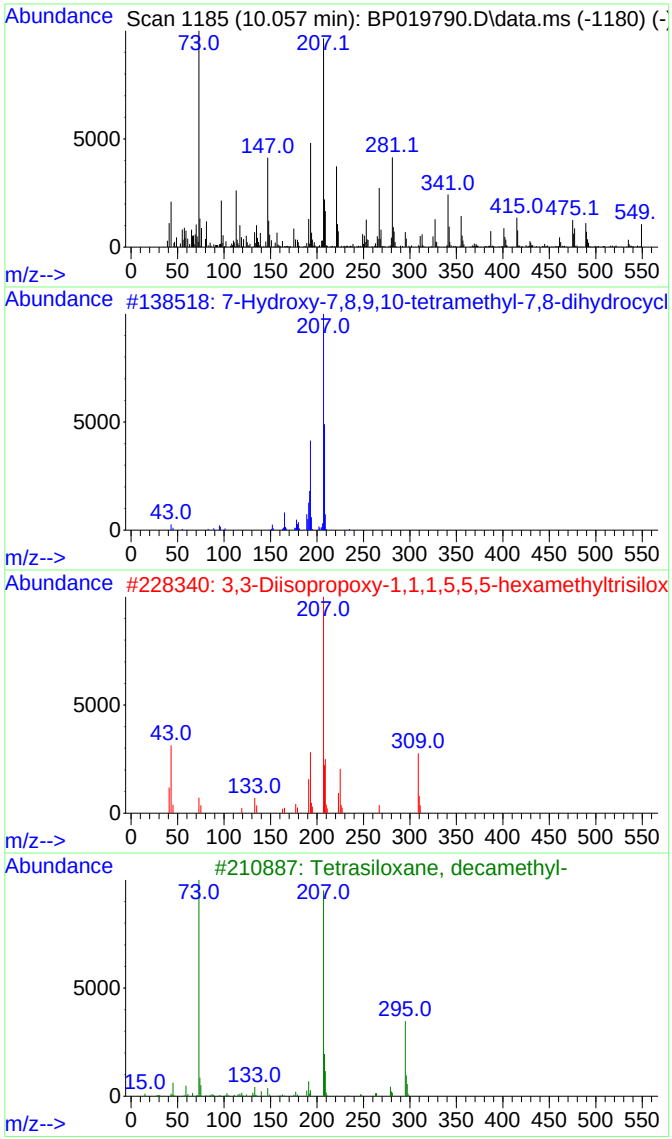
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

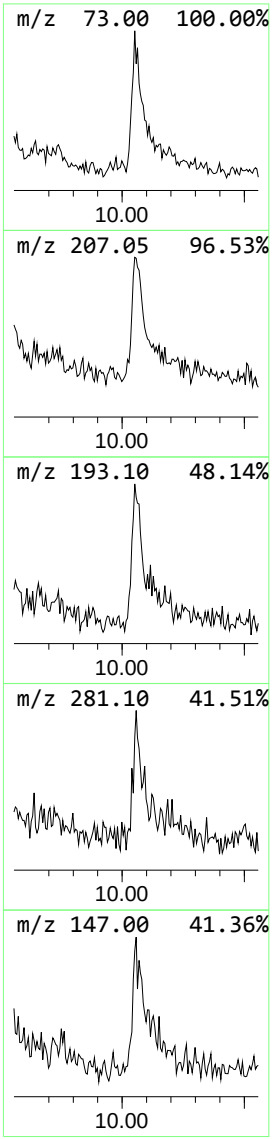
****

Peak Number 13 unknown10.057 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.057	3.23 ng	87860	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hydroxy-7,8,9,10-tetramethyl-7...	252	C18H20O	1000110-34-9	35
2	3,3-Diisopropoxy-1,1,1,5,5,5-hex...	324	C12H32O4Si3	018082-56-9	35
3	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	30
4	1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	30
5	1,4-Bis(trimethylsilyl)benzene	222	C12H22Si2	013183-70-5	30





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

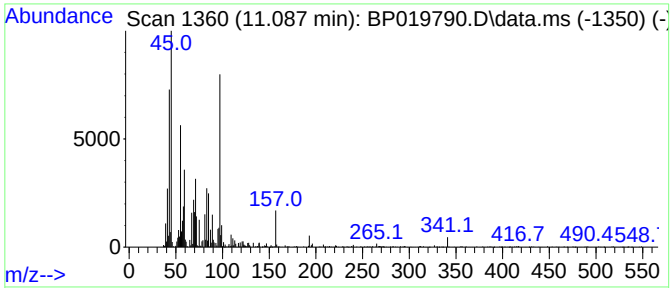
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

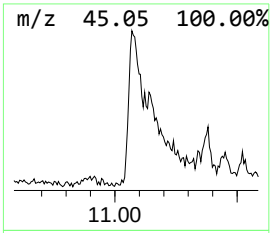
****

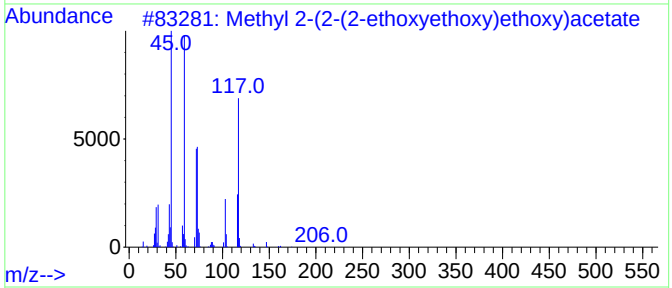
Peak Number 14 unknown11.087 Concentration Rank 17

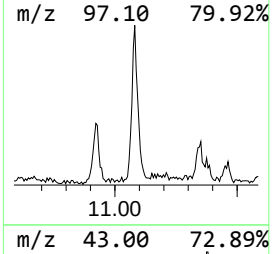
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.087	3.95 ng	107231	Naphthalene-d8	10.698

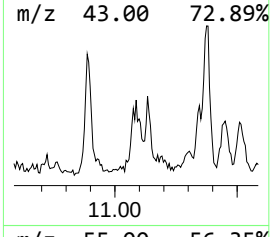
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-(2-(2-ethoxyethoxy)etho...	206	C9H18O5	1000366-78-1	35
2	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	35
3	DL-Glyceraldehyde, dimethyl ether	118	C5H10O3	1010332-93-3	35
4	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	30
5	Triethylene glycol	150	C6H14O4	000112-27-6	27

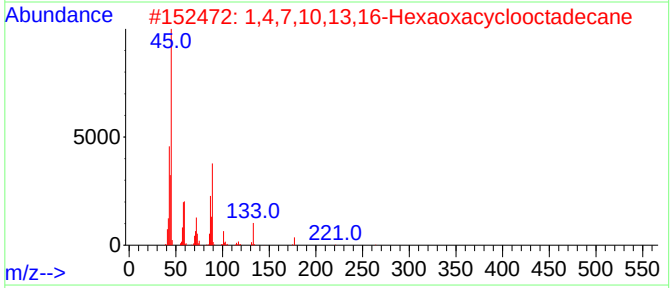


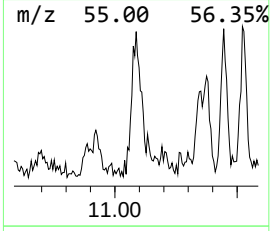


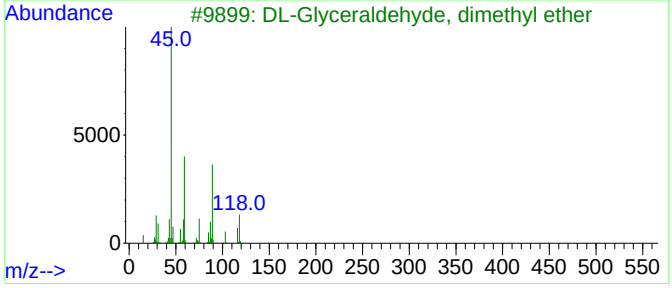


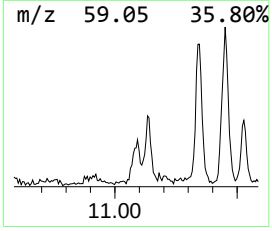












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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
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Instrument :
BNA_P
ClientSampleId :
20240768-AMENDED-COMP-39N-N-3-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

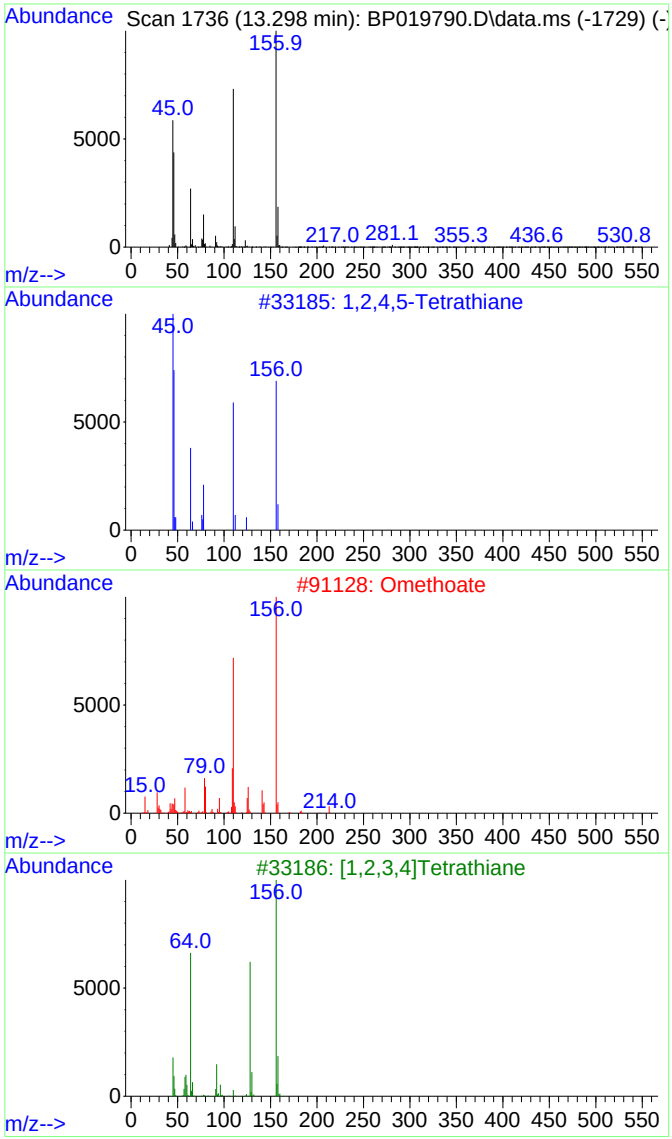
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

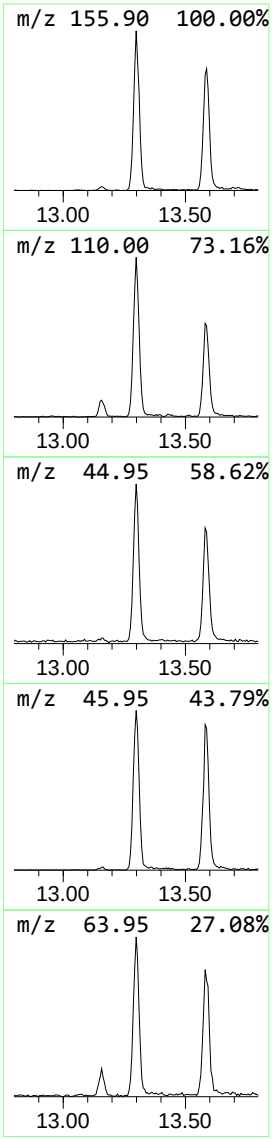
****

Peak Number 15 1,2,4,5-Tetrathiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	5.79 ng	226580	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	94
2	Omethoate	213	C5H12NO4PS	001113-02-6	38
3	[1,2,3,4]Tetrathiane	156	C2H4S4	000290-81-3	38
4	DL-Alanine, N-methyl-N-(byt-3-en...	355	C20H37NO4	1000392-73-6	10
5	Catechol	110	C6H6O2	000120-80-9	10





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

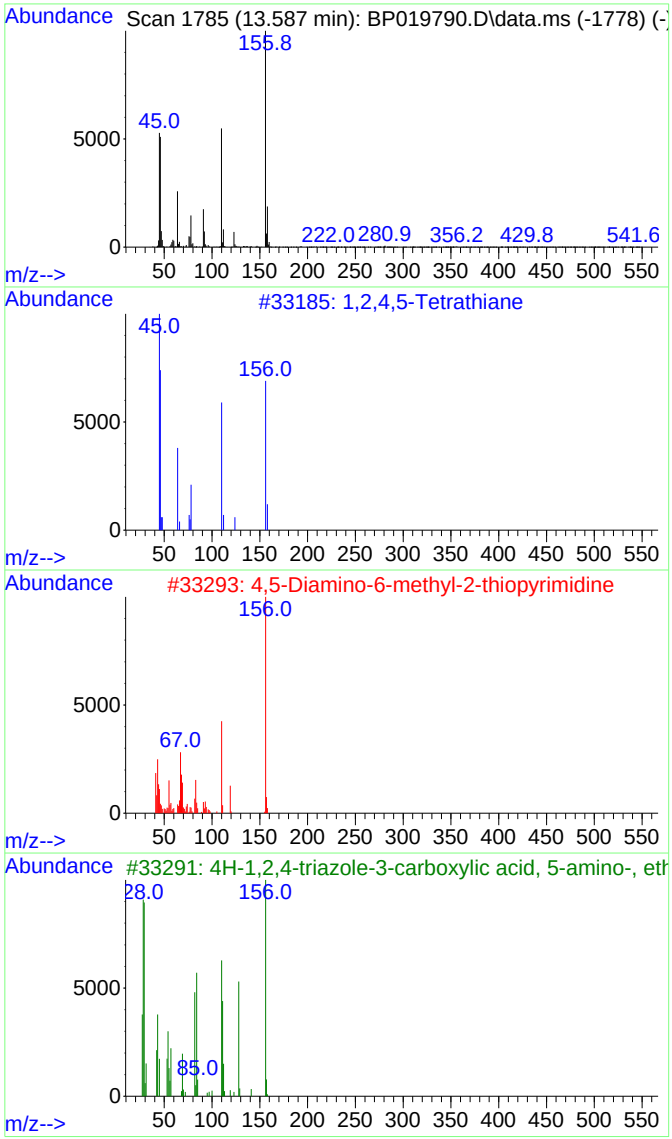
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

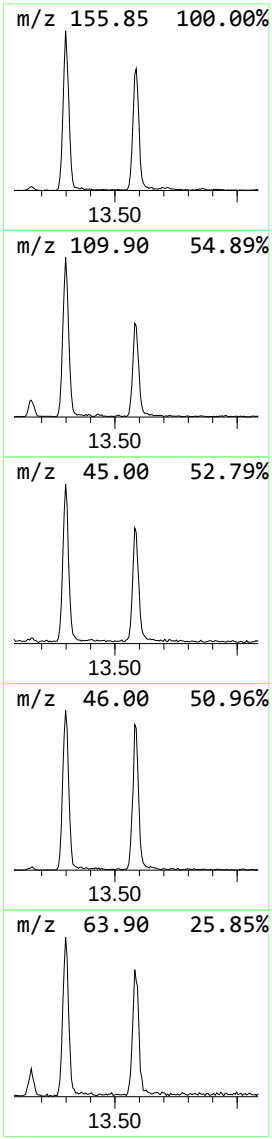
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 unknown13.586 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	4.86 ng	190259	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	94
2	4,5-Diamino-6-methyl-2-thiopyrim...	156	C5H8N4S	006305-99-3	47
3	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	32
4	N-Acetyl-veratramine	451	C29H41NO3	1010256-72-3	12
5	DL-Alanine, N-methyl-N-(byt-3-en...	341	C19H35NO4	1000392-73-5	12





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Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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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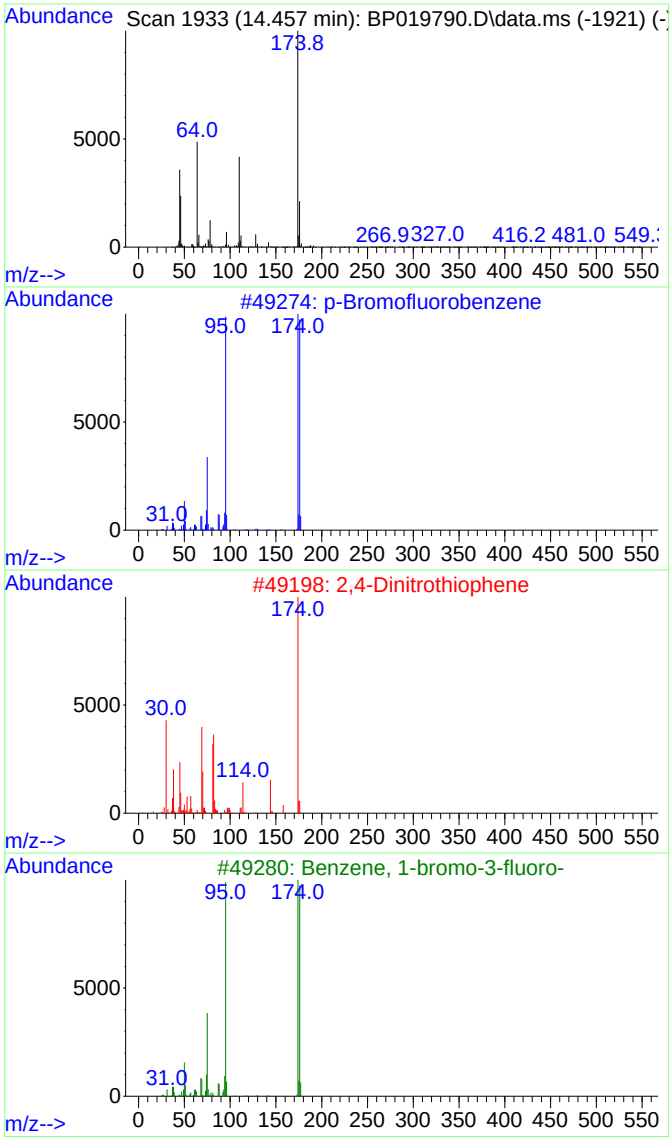
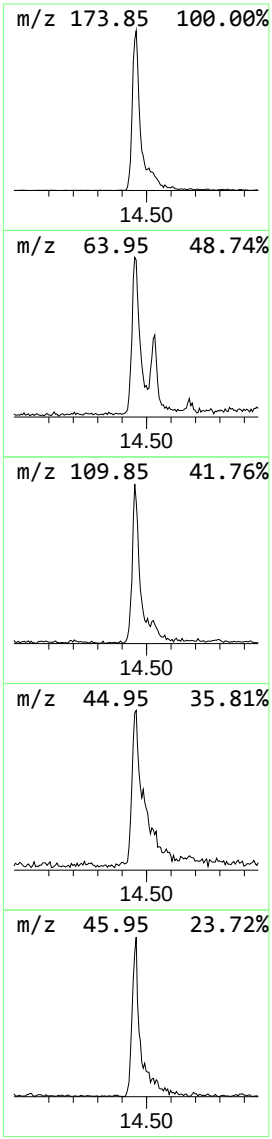
Peak Number 17 unknown14.457 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	4.83 ng	188968	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	9
2	2,4-Dinitrothiophene	174	C4H2N2O4S	005347-12-6	9
3	Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	9
4	2-Fluoro-4-phenylpyrimidine	174	C10H7FN2	038953-34-3	7
5	4-Methyl-5-phenyl-imidazol-2(3H)...	174	C10H10N2O	1000147-06-1	7





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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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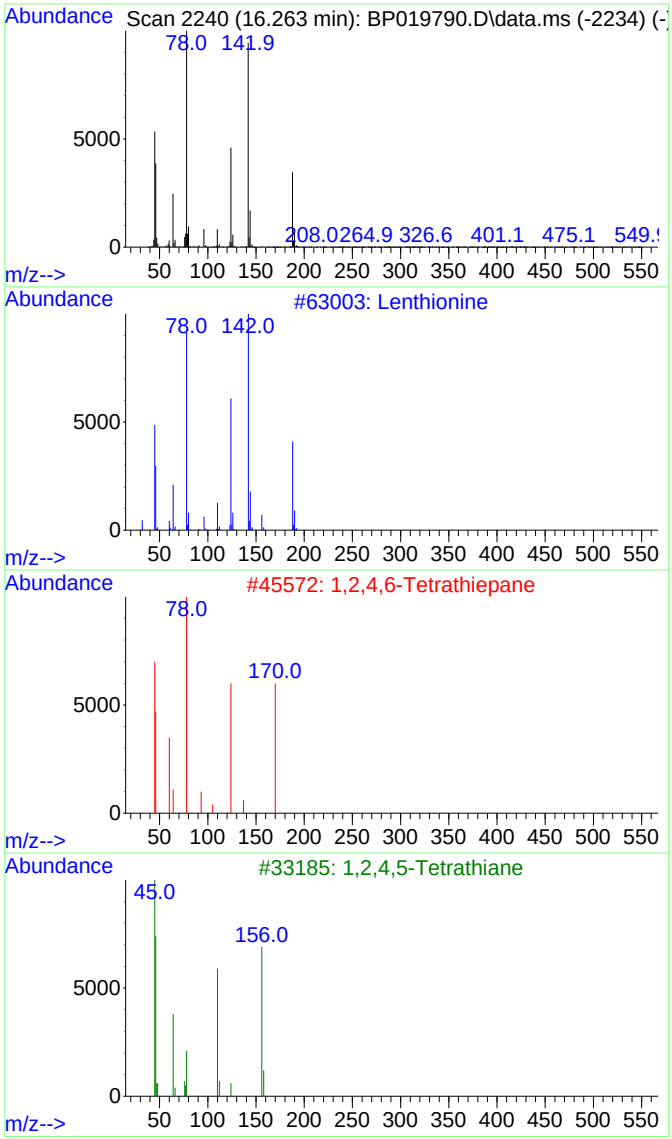
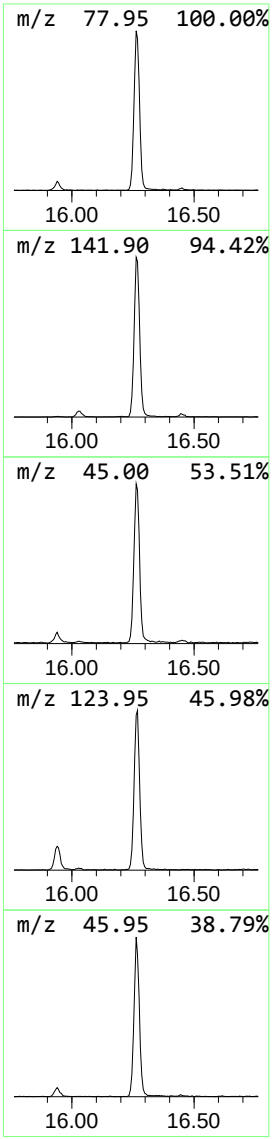
Peak Number 18 Lenthionine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.263	13.46 ng	704728	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	86
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	10
4	1,3-Benzenedithiol	142	C6H6S2	000626-04-0	9
5	1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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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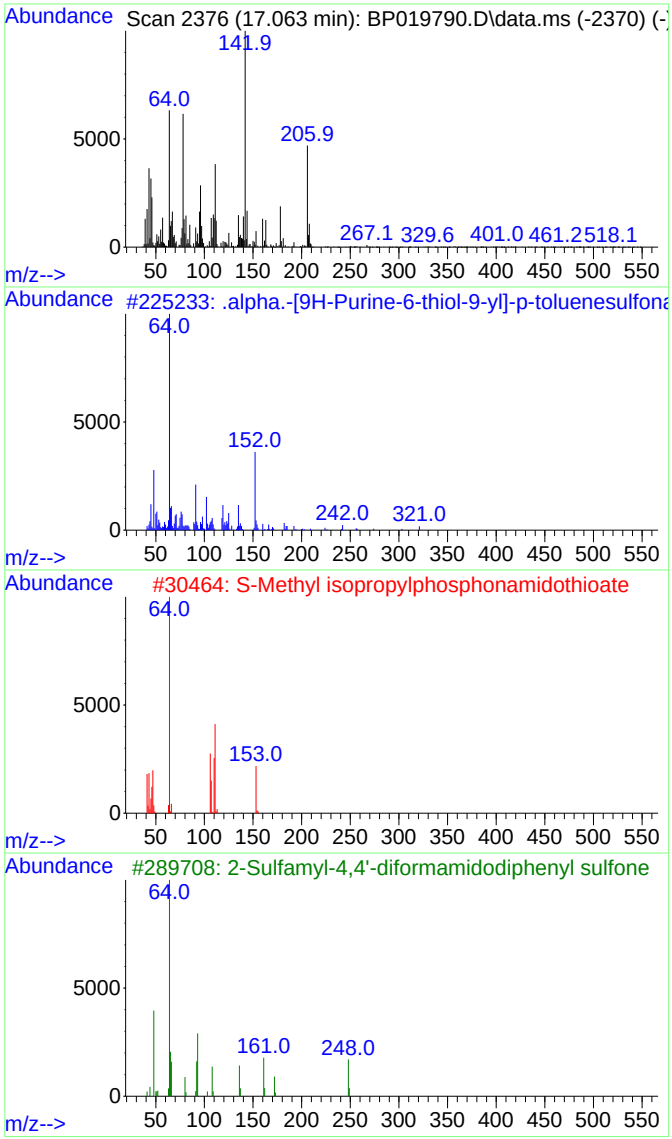
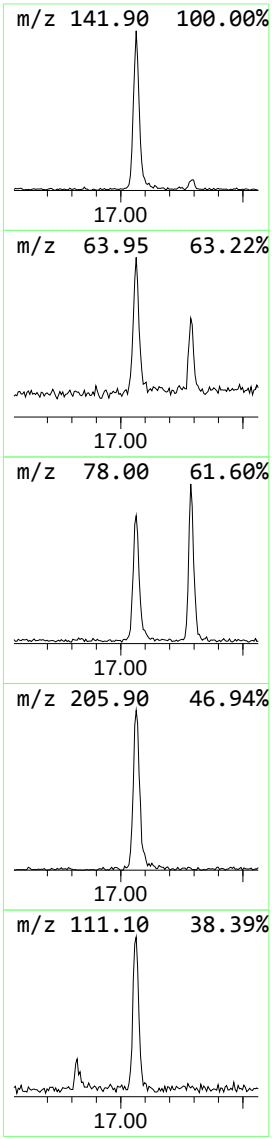
Peak Number 19 unknown17.063 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.063	4.21 ng	220491	Phenanthrene-d10	17.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-[9H-Purine-6-thiol-9-yl]...	321	C12H11N5O2S2	019271-00-2	22
2	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	16
3	2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	12
4	4-Amino-1-methyl-3-nitropyrazole	142	C4H6N4O2	039205-76-0	11
5	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	10





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Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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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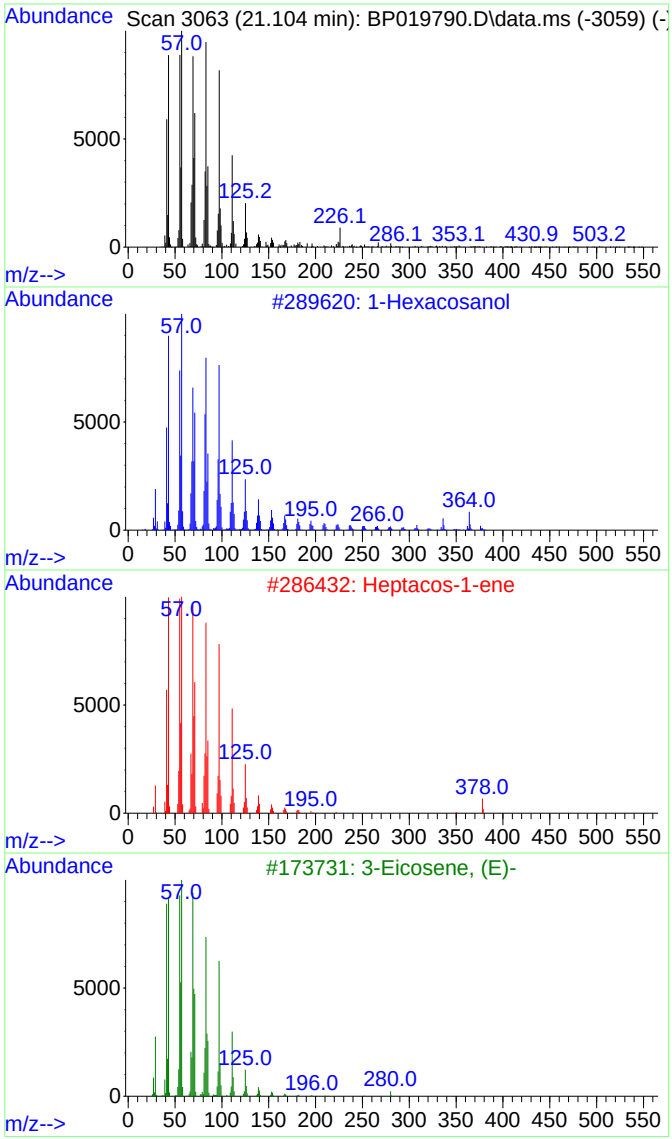
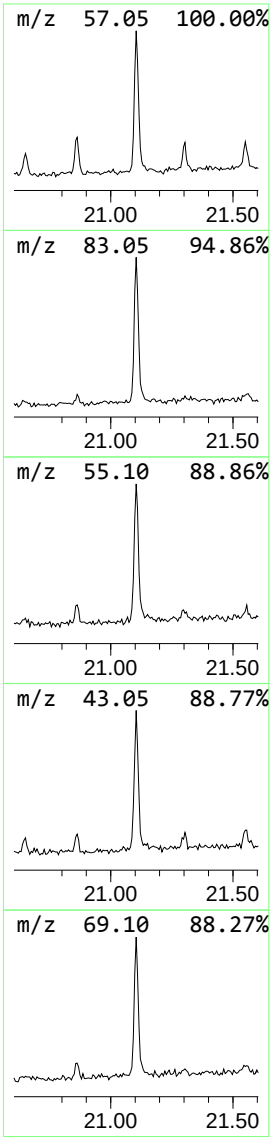
Peak Number 20 1-Hexacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	4.93 ng	324097	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	94
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	Pentacos-1-ene	350	C25H50	016980-85-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019790.D
Acq On : 20 Feb 2024 17:36
Operator : MA/JU
Sample : P1523-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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	3.134	163.3	ng	3065860	1	7.899	375361	20.0
2-Butenal, 2-me...	3.746	3.8	ng	71867	1	7.899	375361	20.0
Prenol	4.069	16.2	ng	304141	1	7.899	375361	20.0
2-Butenal, 3-me...	4.246	4.9	ng	92110	1	7.899	375361	20.0
unknown4.458	4.458	5.5	ng	103099	1	7.899	375361	20.0
2-Pentanol, 4-m...	4.640	21.1	ng	396425	1	7.899	375361	20.0
unknown4.693	4.693	13.9	ng	260691	1	7.899	375361	20.0
2-Pentanone, 4-...	5.022	129.4	ng	2429370	1	7.899	375361	20.0
4-Chloro-3-meth...	7.593	5.3	ng	100229	1	7.899	375361	20.0
2(5H)-Furanone,...	8.140	3.7	ng	68773	1	7.899	375361	20.0
unknown8.869	8.869	4.6	ng	85790	1	7.899	375361	20.0
1,2-Benzenediol...	9.434	129.6	ng	3520020	2	10.698	543380	20.0
unknown10.057	10.057	3.2	ng	87860	2	10.698	543380	20.0
unknown11.087	11.087	4.0	ng	107231	2	10.698	543380	20.0
1,2,4,5-Tetrath...	13.298	5.8	ng	226580	3	14.534	782851	20.0
unknown13.586	13.586	4.9	ng	190259	3	14.534	782851	20.0
unknown14.457	14.457	4.8	ng	188968	3	14.534	782851	20.0
Lenthionine	16.263	13.5	ng	704728	4	17.292	1047240	20.0
unknown17.063	17.063	4.2	ng	220491	4	17.292	1047240	20.0
1-Hexacosanol	21.104	4.9	ng	324097	5	21.380	1313780	20.0