LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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: BP019793.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	3	7	20	rVB	1964585	2240339	50.73%	9.280%
2	3.746	108	112	119	rBV2	31222	53907	1.22%	0.223%
3	4.069	161	167	176	rBV2	139518	228723	5.18%	0.947%
4	4.246	191	197	203	rBV	43114	67217	1.52%	0.278%
5	4.452	228	232	243	rVB	52320	80744	1.83%	0.334%
6	4.640	259	264	269	rVV	209263	302784	6.86%	1.254%
7	4.693	269	273	284	rVB	124823	199775	4.52%	0.827%
8	5.016	322	328	337	rBV	825477	1160072	26.27%	4.805%
9	5.469	398	405	422	rBV	557179	864032	19.57%	3.579%
10	5.793	455	460	466	rBV2	30441	49044	1.11%	0.203%
11	6.099	502	512	515	rBV2	22711	50448	1.14%	0.209%
12	6.722	614	618	624	rBV5	24179	61100	1.38%	0.253%
13	7.069	669	677	684	rBV	657401	1095176	24.80%	4.536%
14	7.593	761	766	772	rBV2	42721	73504	1.66%	0.304%
15	7.893	812	817	824	rVB	228271	372389	8.43%	1.542%
16	8.140	853	859	863	rBV2	28059	51145	1.16%	0.212%
17	8.869	977	983	988	rBV4	31480	75001	1.70%	0.311%
18	9.063	1009	1016	1028	rBV	502931	872908	19.77%	3.616%
19	9.357	1057	1066	1071	rBV6	21341	59314	1.34%	0.246%
20	9.428	1071	1078	1088	rVV	854842	1593207	36.08%	6.599%
21	10.057	1179	1185	1191	rBV3	23376	60099	1.36%	0.249%
22	10.693	1285	1293	1309	rBV	285706	537783	12.18%	2.228%
23	11.087	1351	1360	1365	rBV7	24767	68699	1.56%	0.285%
24	11.446	1415	1421	1429	rVB2	29380	52842	1.20%	0.219%
25	13.157	1705	1712	1730	rBV	1382615	2163484	48.99%	8.961%
26	13.298	1730	1736	1743	rVB	111614	194501	4.40%	0.806%
27	13.581	1778	1784	1791	rBV	51481	94103	2.13%	0.390%
28	14.451	1924	1932	1940	rBV	62258	138642	3.14%	0.574%
29	14.534	1940	1946	1960	rVB	471923	786714	17.81%	3.259%
30	15.145	2040	2050	2070	rBV4	39398	173248	3.92%	0.718%
31	16.028	2193	2200	2219	rBV	600260	975832	22.10%	4.042%
32	16.263	2234	2240	2252	rBV	355864	585018	13.25%	2.423%
33	17.057	2370	2375	2389	rVB2	132262	232874	5.27%	0.965%
34	17.286	2408	2414	2421	rBV	732114	1085267	24.58%	4.495%
35	18.181	2562	2566	2573	rBV2	62973	98089	2.22%	0.406%
36	19.298	2753	2756	2763	rVB	42680	56423	1.28%	0.234%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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	19.645	2813	2815	2819	rVB	37243	46206	1.05%	0.191%
38	19.857	2845	2851	2858	rBV	3386433	4416090	100.00%	18.292%
39	20.857	3019	3021	3027	rVB	51415	53591	1.21%	0.222%
40	21.104	3059	3063	3069	rVB	242018	316162	7.16%	1.310%
41	21.380	3105	3110	3115	rBV	923998	1249941	28.30%	5.177%
42	23.798	3514	3521	3530	rVB	573982	1206147	27.31%	4.996%

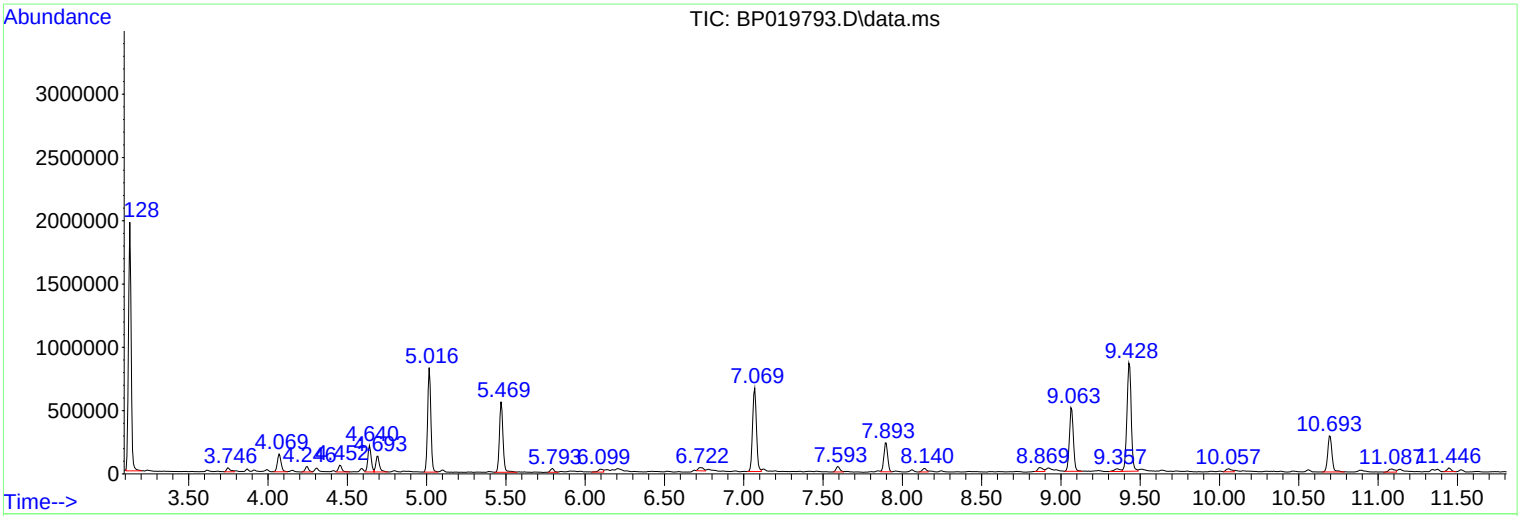
Sum of corrected areas: 24142584

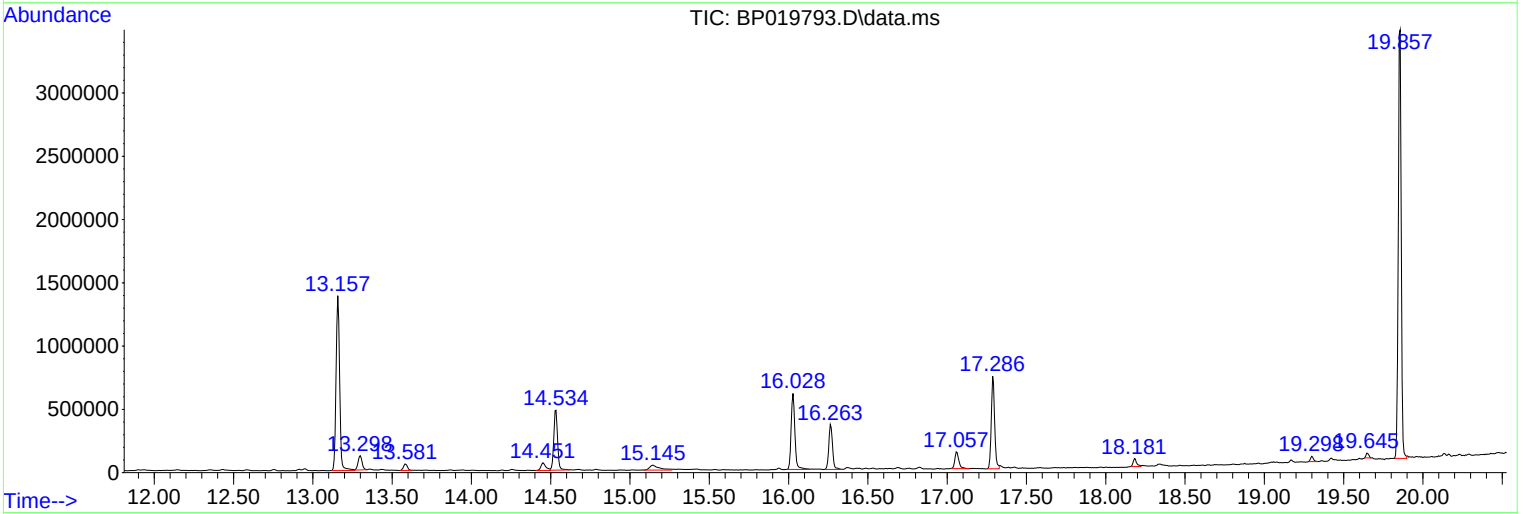
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

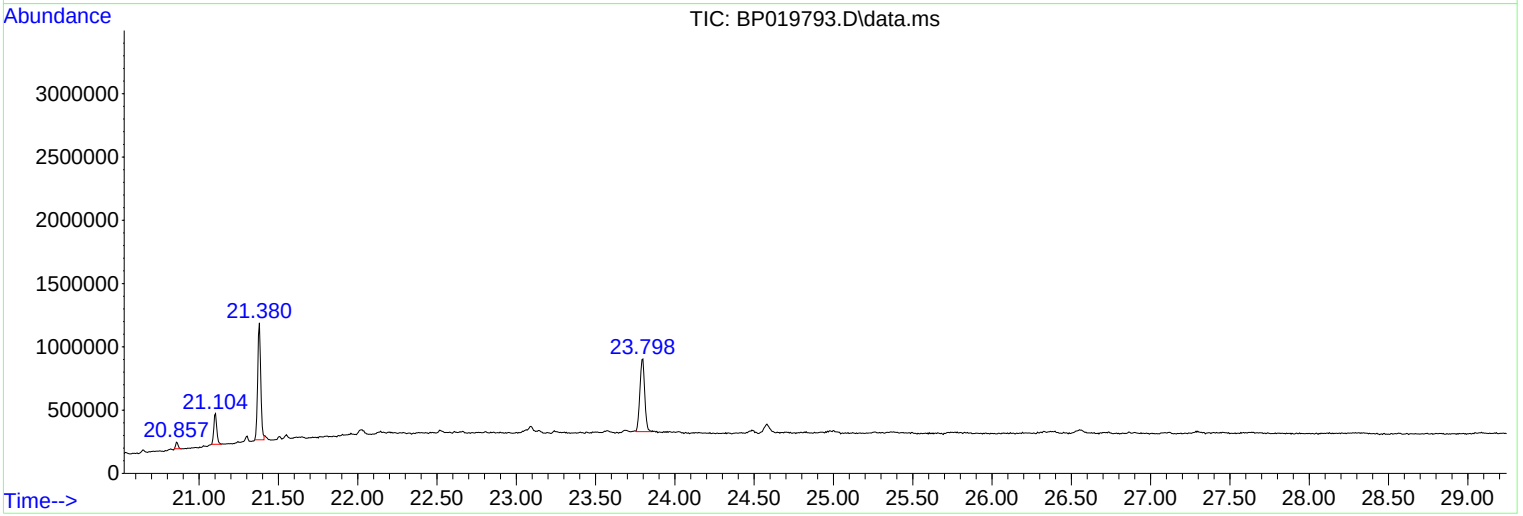
Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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 : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

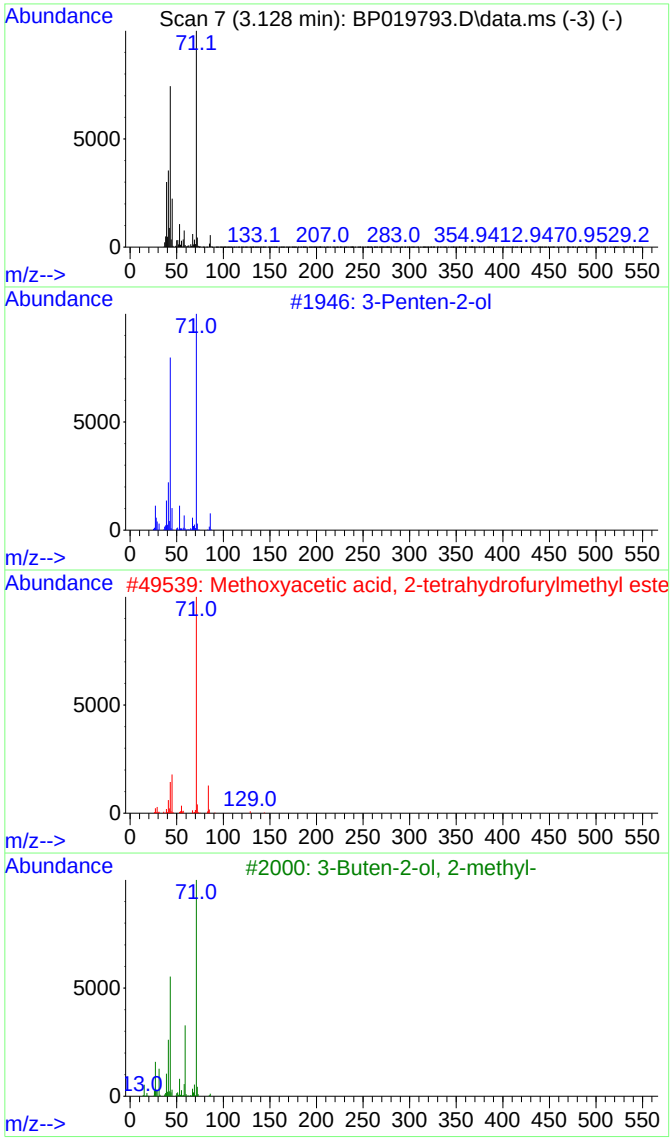
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

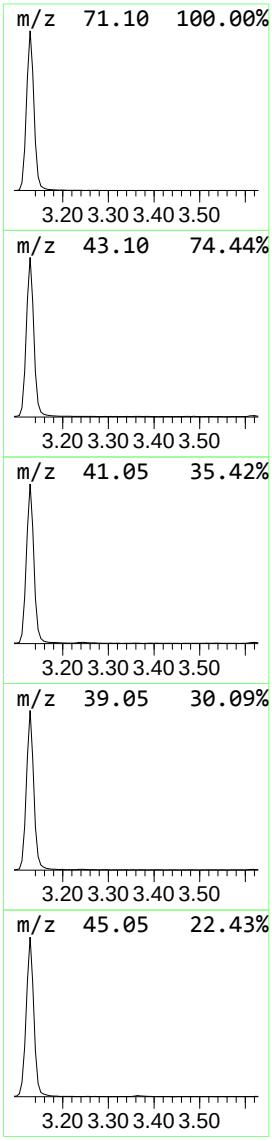
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	120.32 ng	2240340	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	87
2	Methoxyacetic acid, 2-tetrahydro...	174	C8H14O4	1000282-41-3	53
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
4	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	50
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

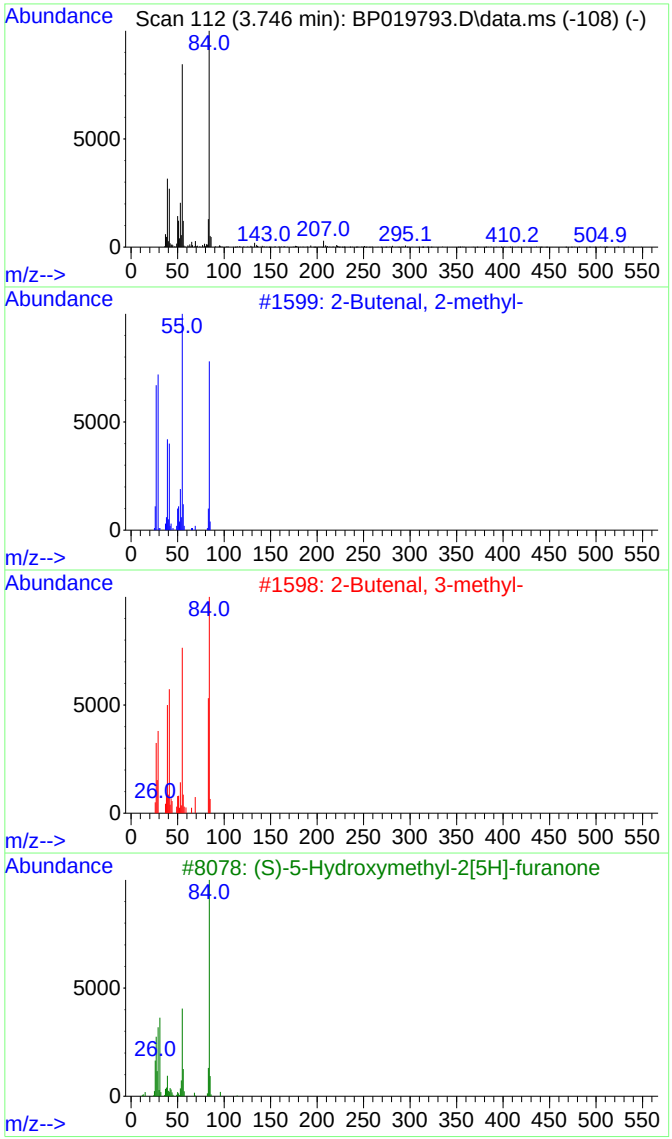
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

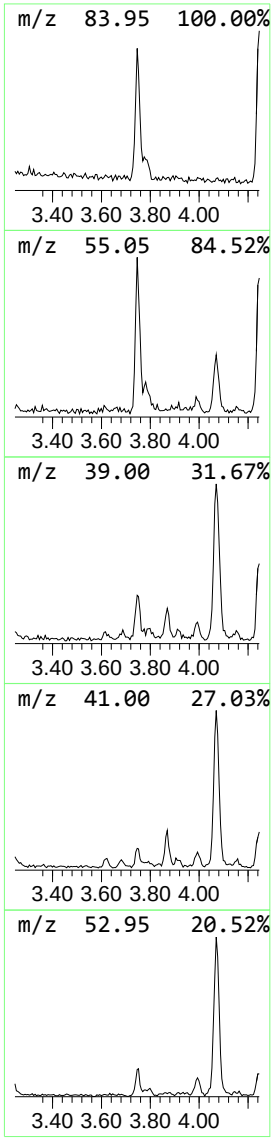
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.746	2.90 ng	53907	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	91
2	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	87
3	(S)-5-Hydroxymethyl-2[5H]-furanone	114	C5H6O3	078508-96-0	50
4	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	50
5	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

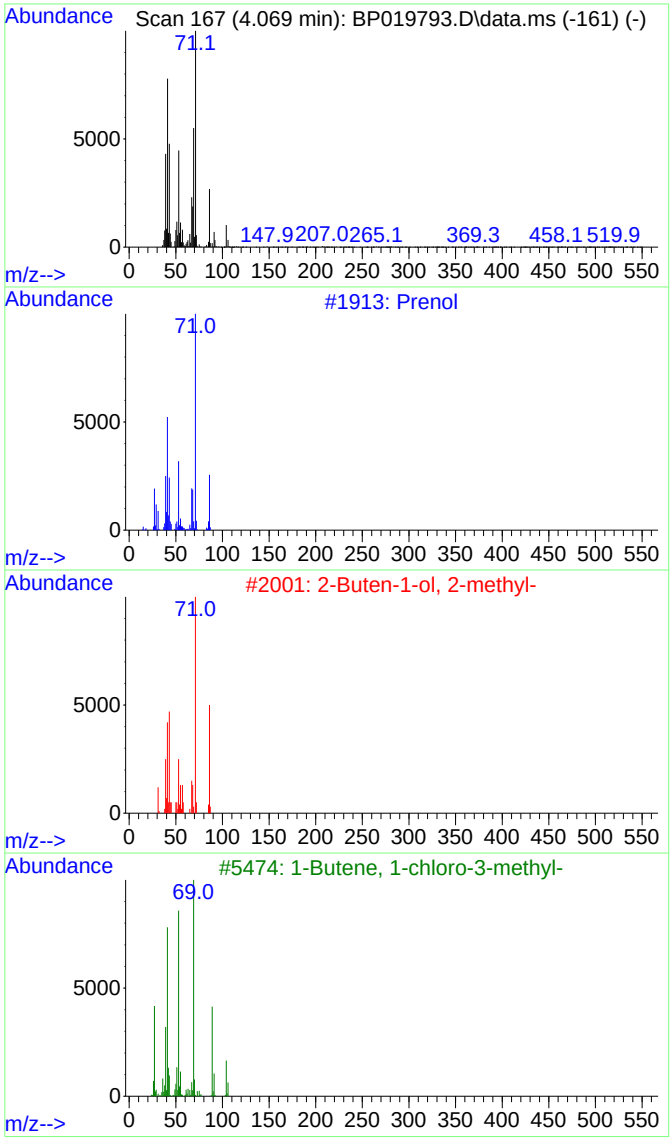
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

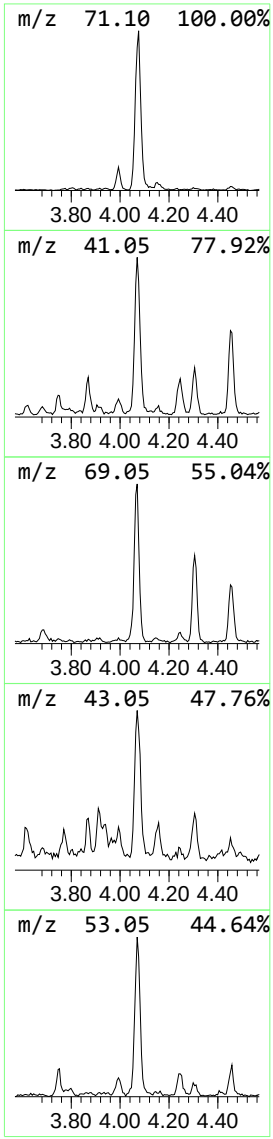
****

Peak Number 3 Prenol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.069	12.28 ng	228723	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	81
2	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	38
3	1-Butene, 1-chloro-3-methyl-	104	C5H9Cl	023010-00-6	38
4	2-Butyne, 1-methoxy-	84	C5H8O	002768-41-4	32
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

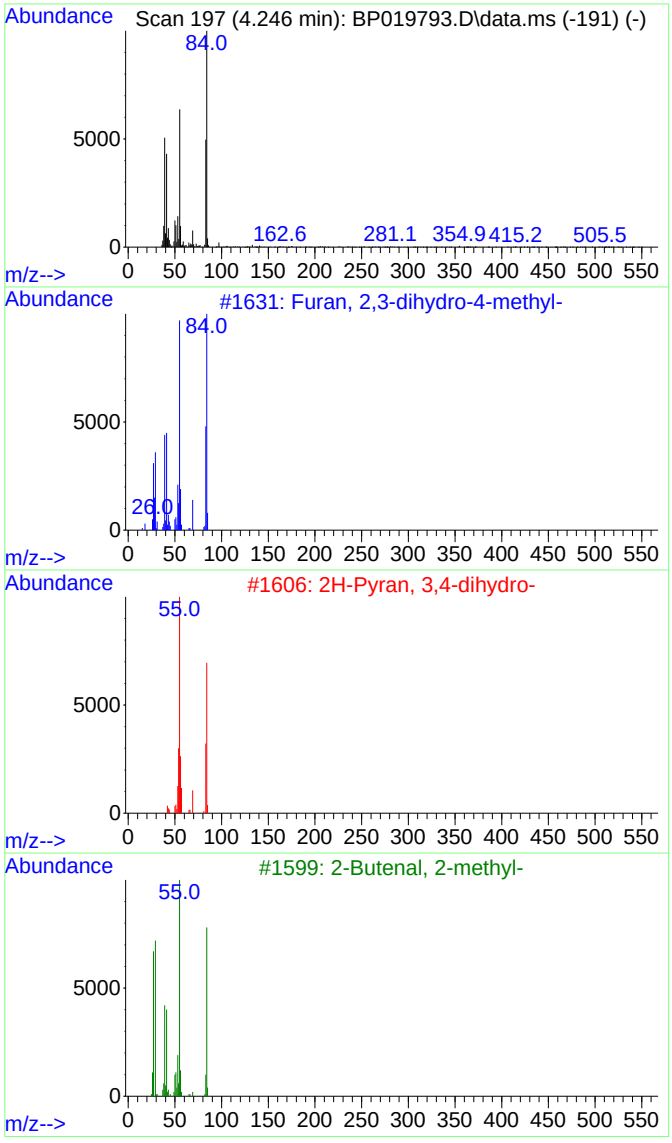
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

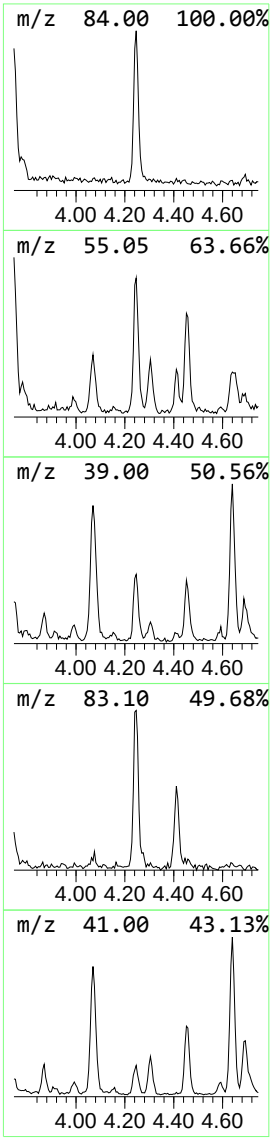
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Furan, 2,3-dihydro-4-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.246	3.61 ng	67217	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	64
2	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	59
3	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	50
4	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	50
5	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

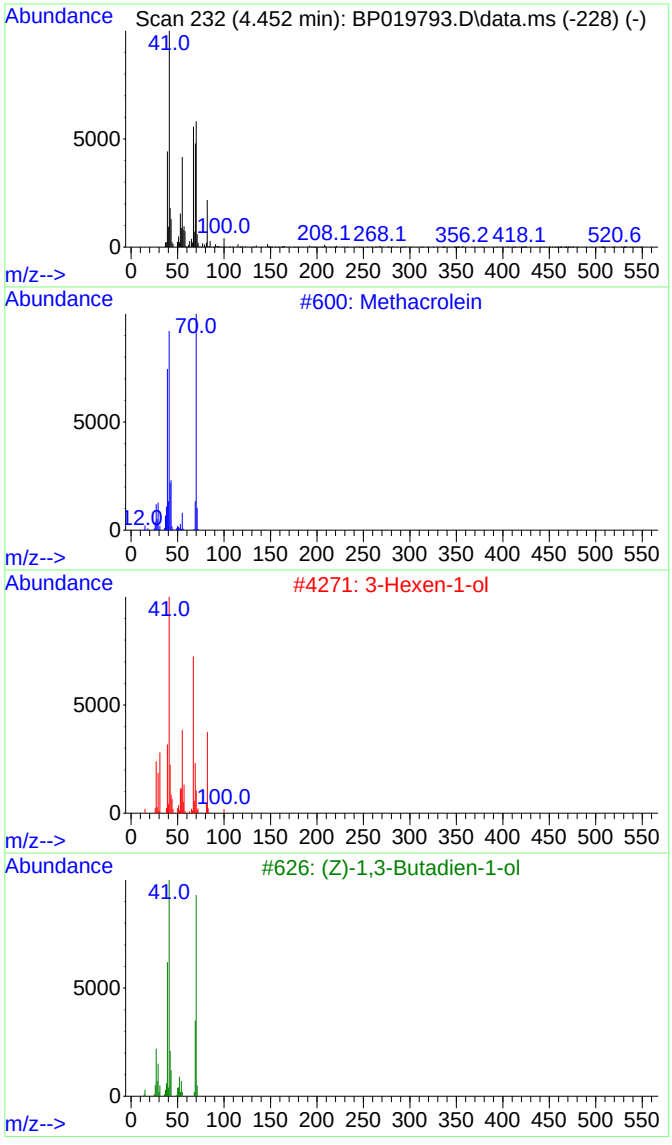
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

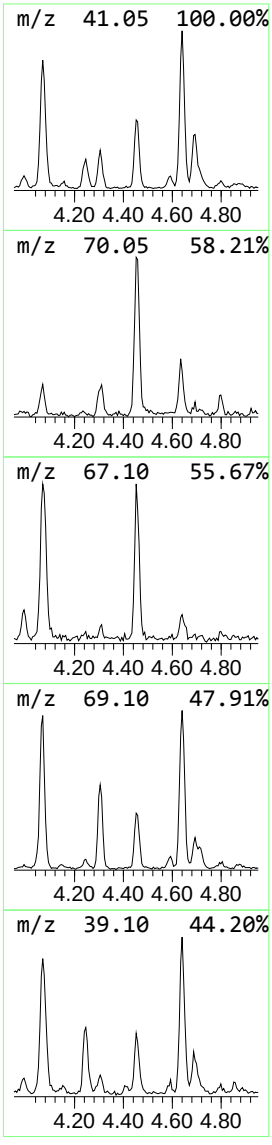
****

Peak Number 5 unknown4.452 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	4.34 ng	80744	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methacrolein	70	C4H6O	000078-85-3	43
2	3-Hexen-1-ol	100	C6H12O	000544-12-7	38
3	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	38
4	4-Hexen-1-ol, (E)-	100	C6H12O	000928-92-7	38
5	3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

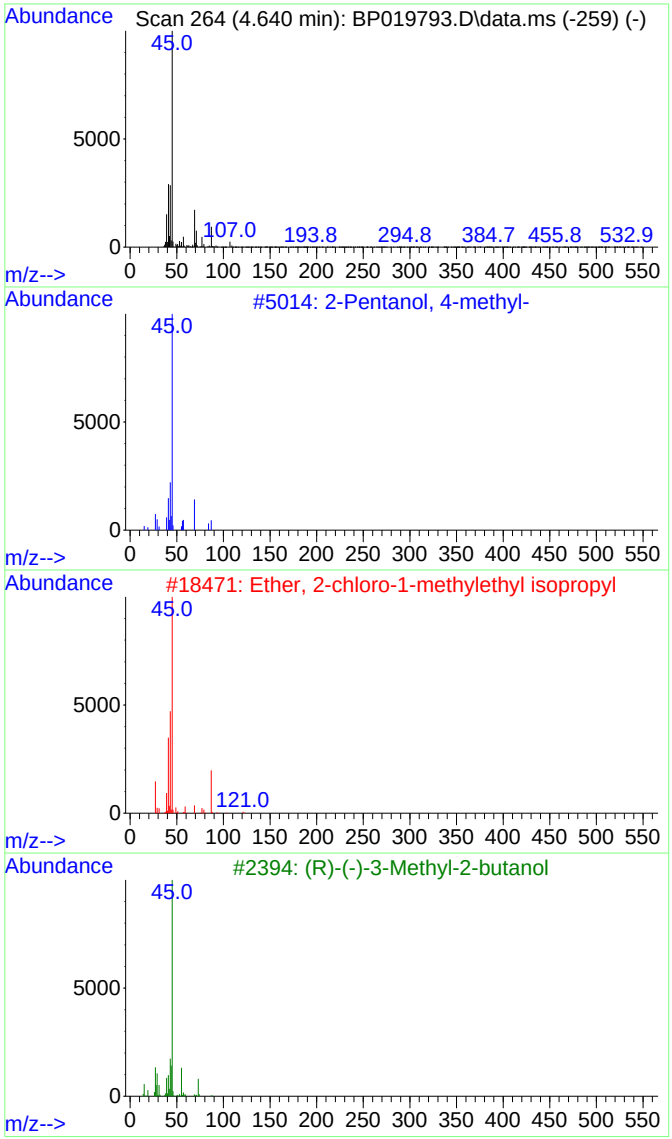
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

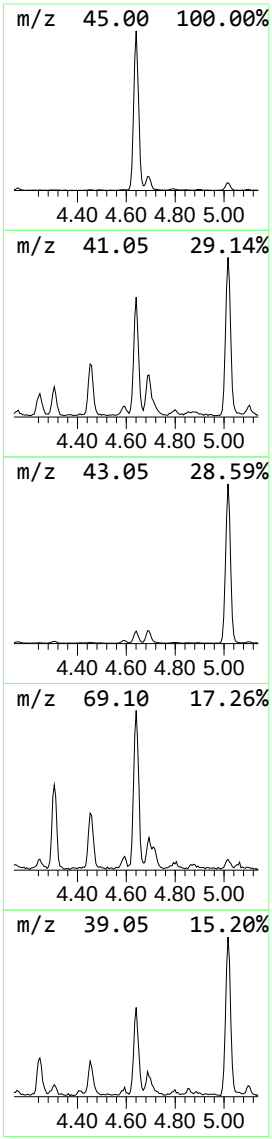
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	16.26 ng	302784	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2	Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	72
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	42
4	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
5	2-Hexanol	102	C6H14O	000626-93-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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

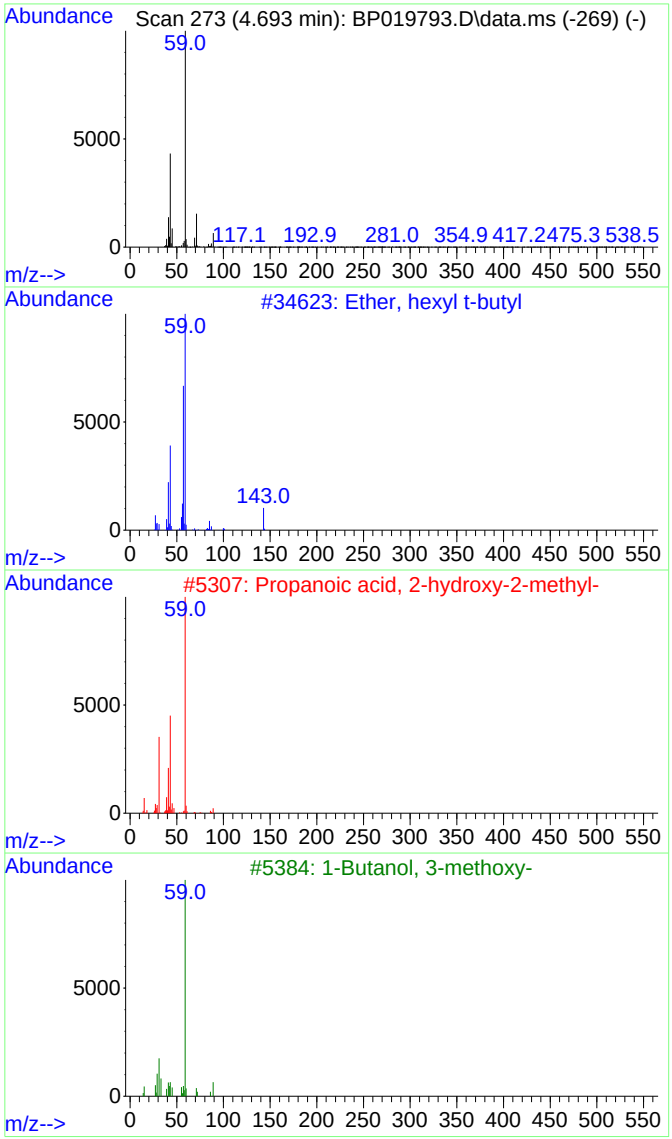
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

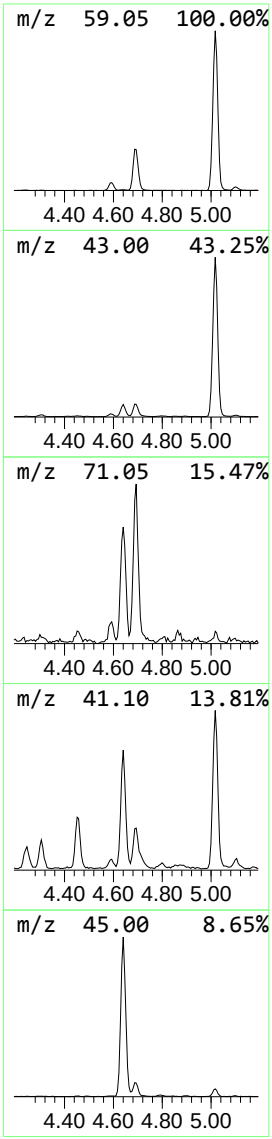
****

Peak Number 7 unknown4.693 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.693	10.73 ng	199775	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ether, hexyl t-butyl	158	C10H22O	069775-79-7	45
2	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	42
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	39
4	1-(1-Methoxypropan-2-yloxy)propa...	244	C9H15F3O4	1010367-08-7	38
5	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

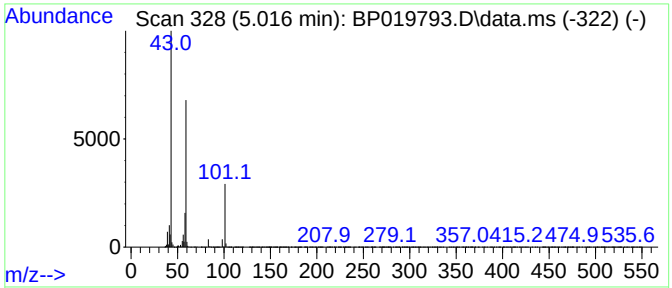
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

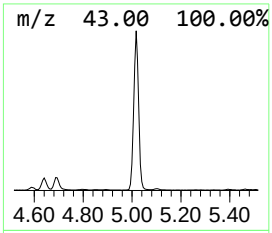
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

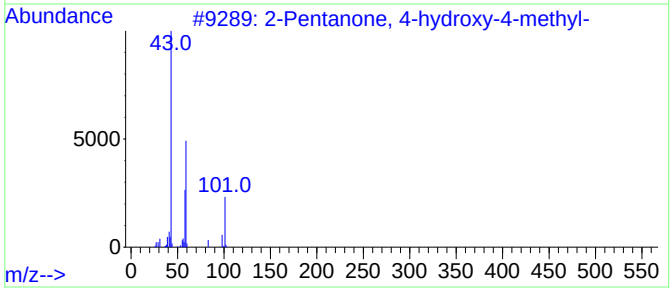
****
Peak Number 8 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

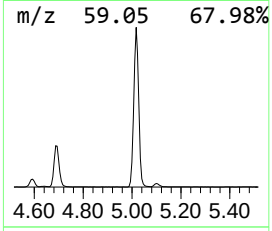
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	62.30 ng	1160070	1,4-Dichlorobenzene-d4	7.893

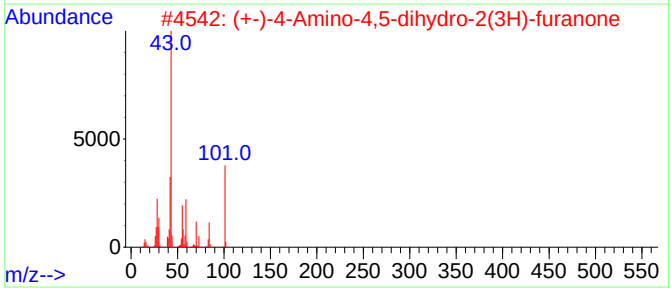
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

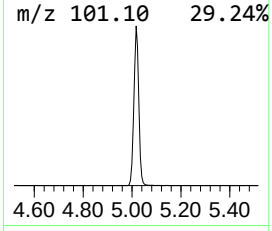


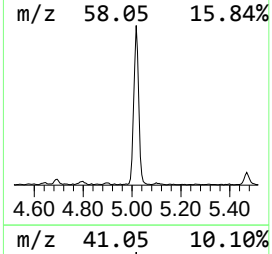


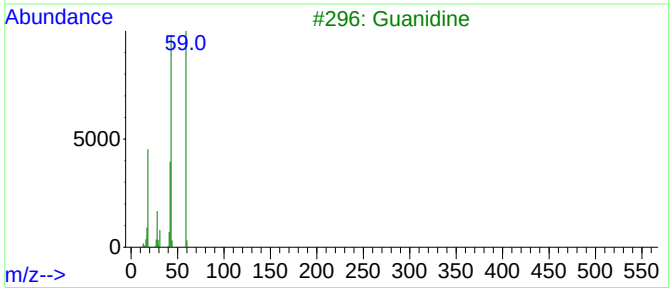


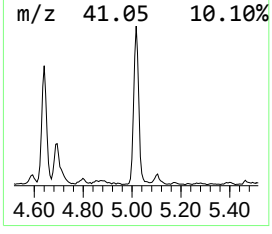












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Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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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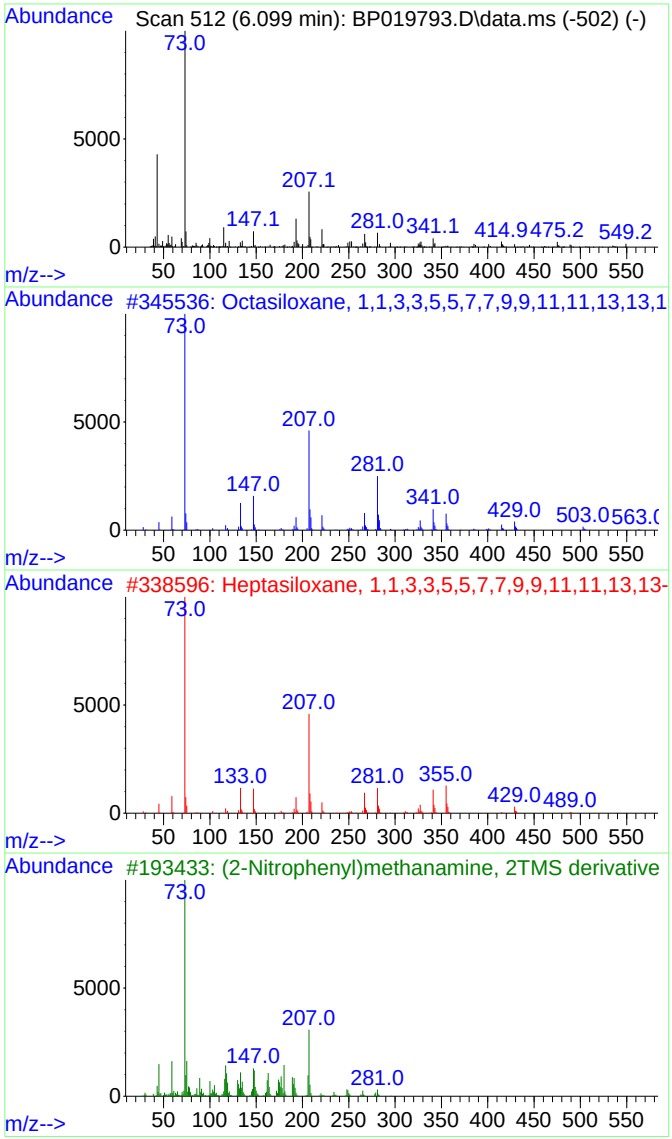
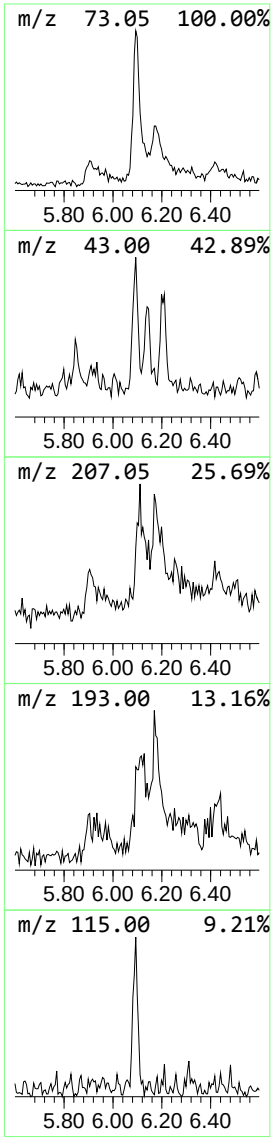
Peak Number 9 unknown6.099 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.099	2.71 ng	50448	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	42
2	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	40
3	(2-Nitrophenyl)methanamine, 2TMS...	296	C13H24N2O2Si2	1000478-84-5	38
4	tert-Butyldimethylsilyl 2-(N-(te...	505	C23H51NO3SSi3	1000417-43-9	22
5	Sulfamic acid, 3TBDMS derivative	439	C18H45NO3SSi3	1000366-59-2	16





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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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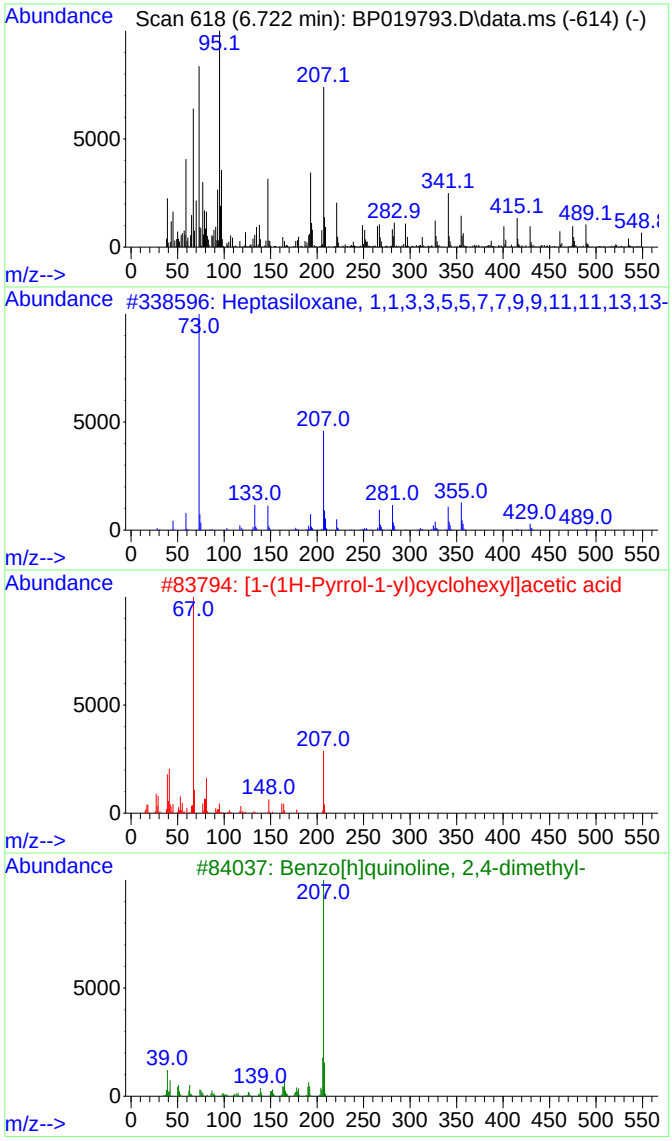
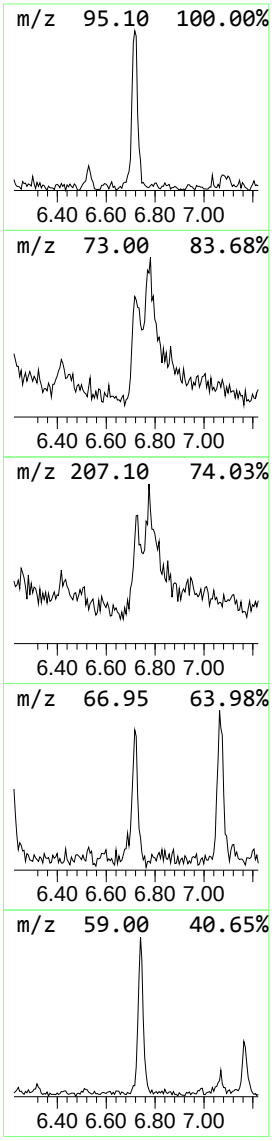
Peak Number 10 unknown6.722 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	3.28 ng	61100	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	25
2	[1-(1H-Pyrrol-1-yl)cyclohexyl]ac...	207	C12H17NO2	1000460-17-9	22
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	20
4	2-Hydroxy-4-methoxynicotinonitri...	222	C10H14N2O2Si	1000484-72-7	20
5	6-Chloro-1-ethyl-4-oxoquinoline-...	251	C12H10ClNO3	066176-24-7	18





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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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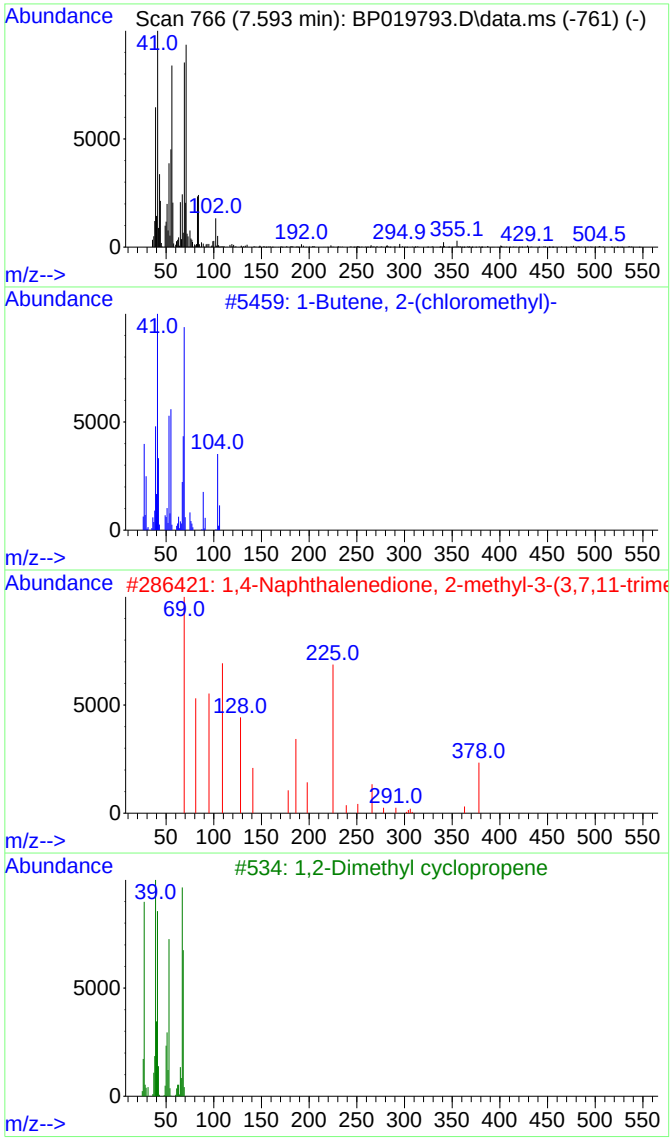
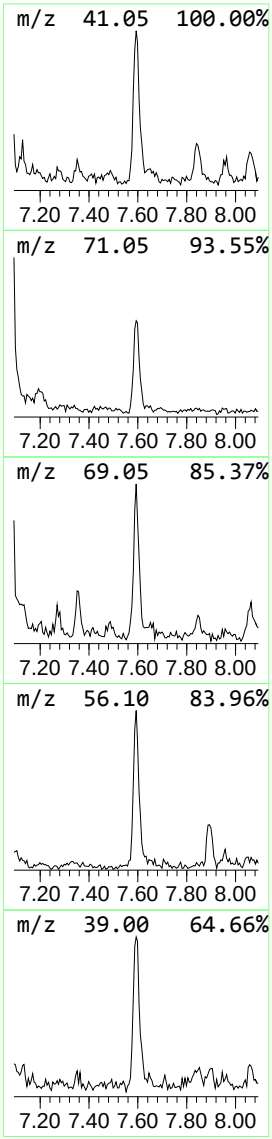
Peak Number 11 unknown7.593 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.593	3.95 ng	73504	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	43
2	1,4-Naphthalenedione, 2-methyl-3...	378	C26H34O2	056324-32-4	27
3	1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	25
4	Butane, 1-(2,2-dichloro-1-methyl...	194	C9H16Cl2	024551-81-3	22
5	Ethane, isocyanato-	71	C3H5NO	000109-90-0	22





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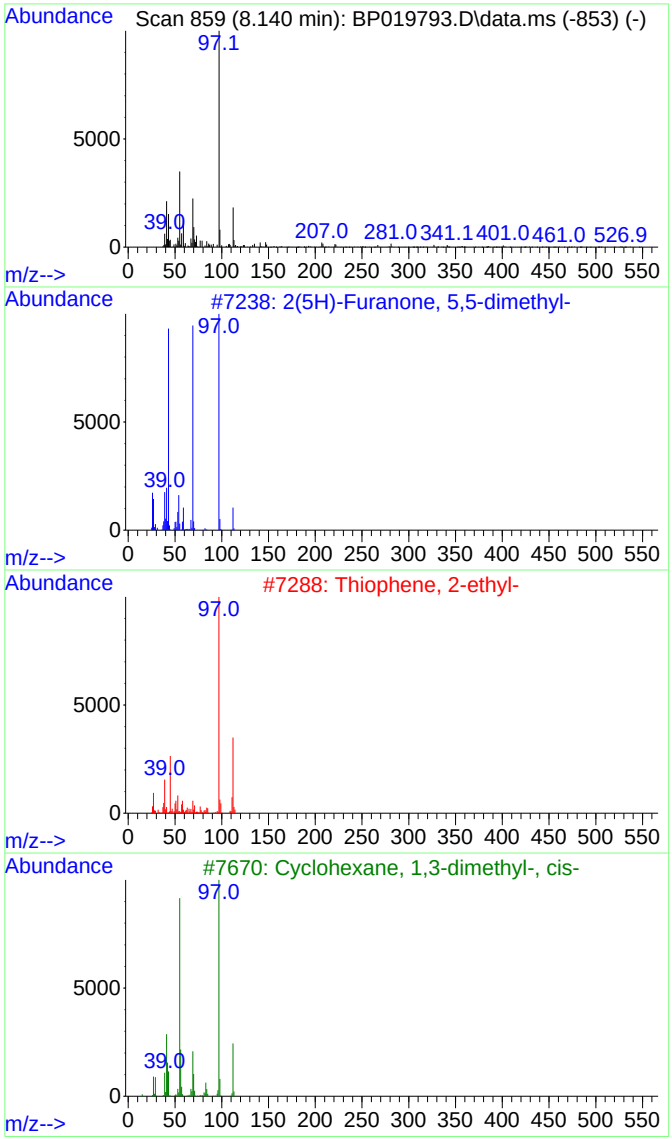
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

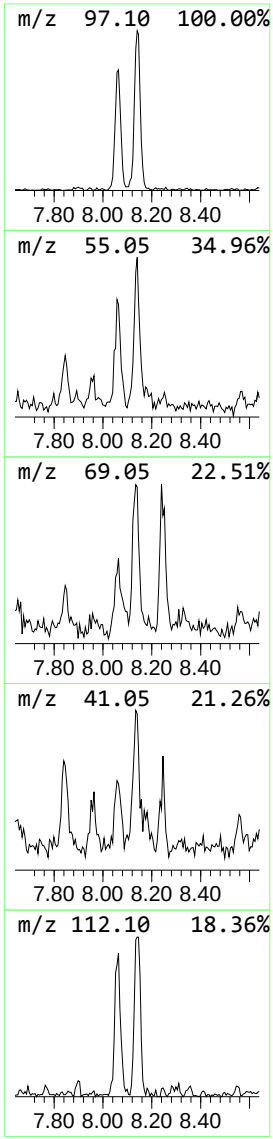
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2(5H)-Furanone, 5,5-dimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	2.75 ng	51145	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	72
2	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	64
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	64
4	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	64
5	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	64





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Misc :
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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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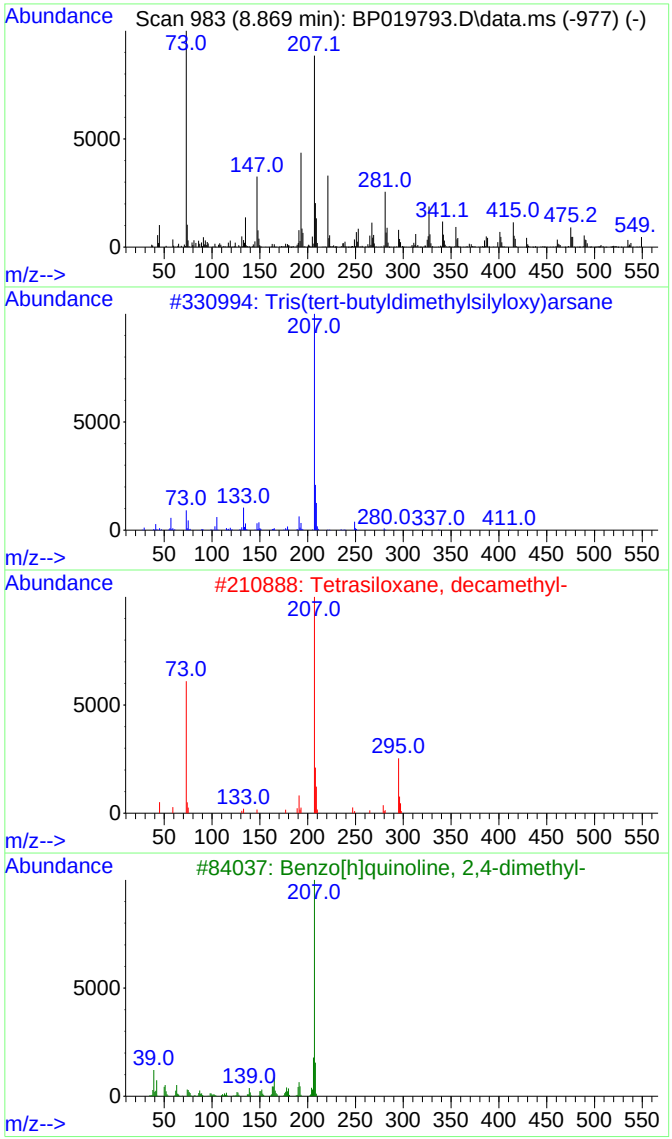
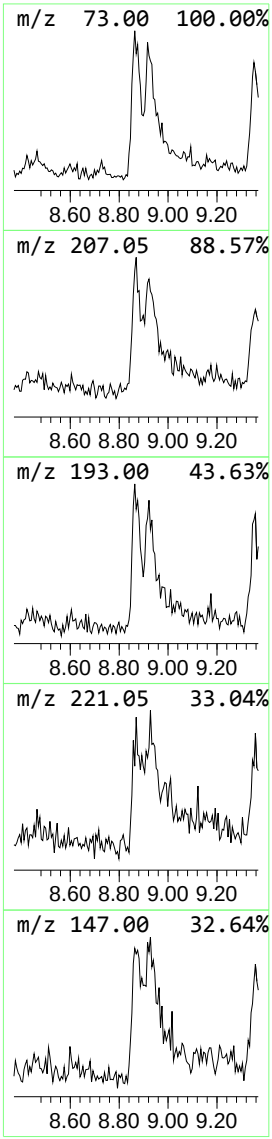
Peak Number 13 unknown8.869 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	4.03 ng	75001	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tris(tert-butyldimethylsilyloxy)...	468	C18H45AsO3Si3	1000366-57-5	43
2	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	43
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5	4-(7-Methyloctyl)phenol, TMS der...	292	C18H32OSi	1000492-40-8	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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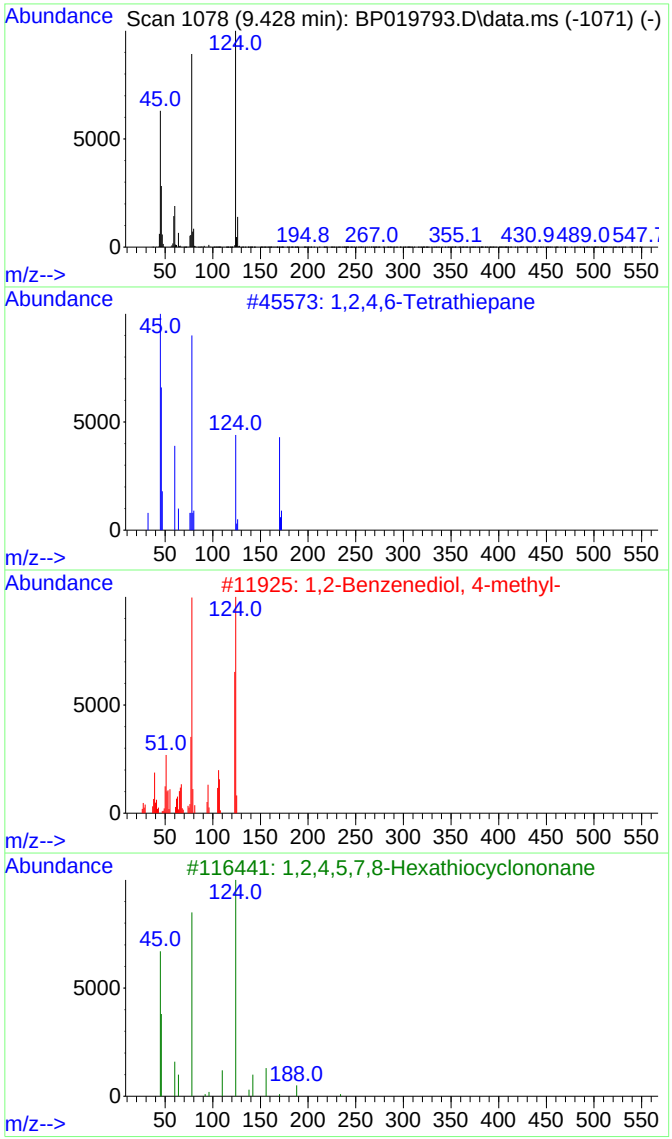
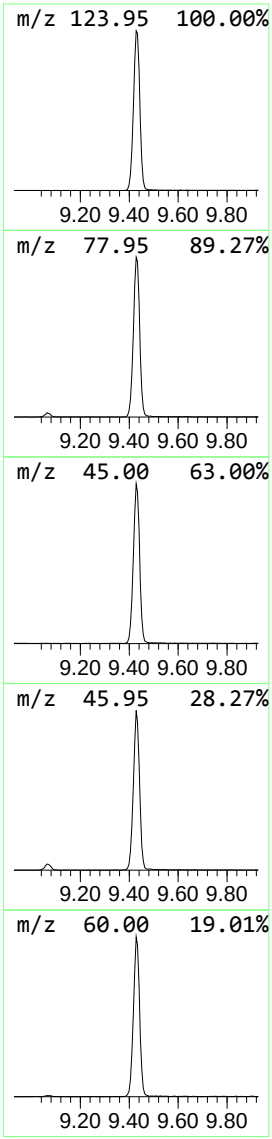
Peak Number 14 1,2,4,6-Tetrathiepane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.428	59.25 ng	1593210	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	59
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
3	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
4	Fumaronitrile	78	C4H2N2	000764-42-1	33
5	Benzene	78	C6H6	000071-43-2	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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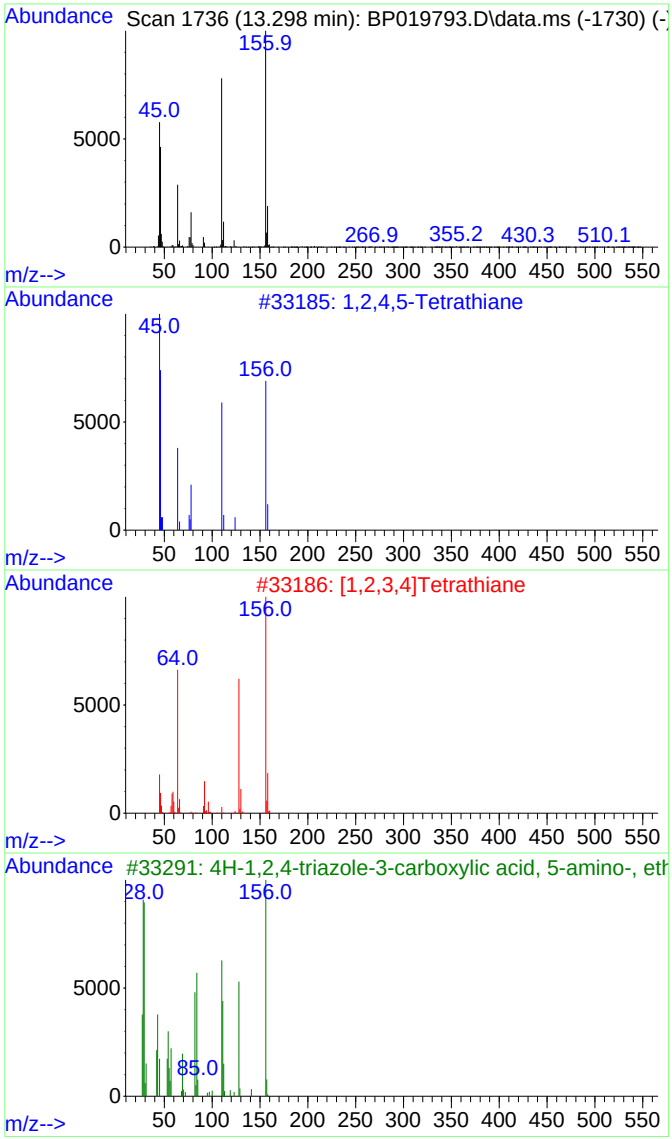
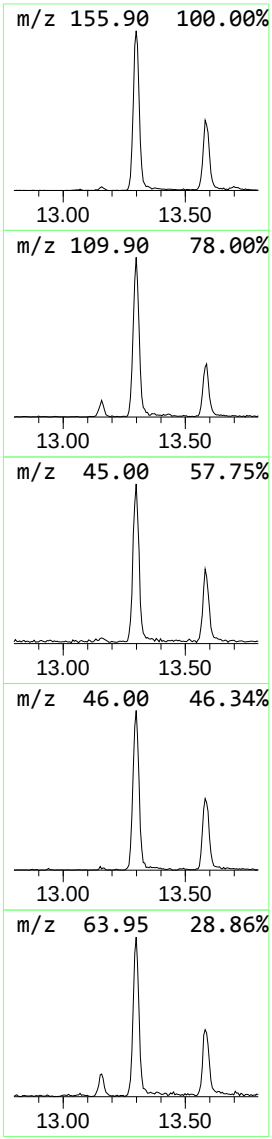
Peak Number 15 1,2,4,5-Tetrathiane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	4.94 ng	194501	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	64
2	[1,2,3,4]Tetrathiane	156	C2H4S4	000290-81-3	38
3	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	37
4	4,5-Diamino-6-methyl-2-thiopyrim...	156	C5H8N4S	006305-99-3	35
5	Omethoate	213	C5H12NO4PS	001113-02-6	28





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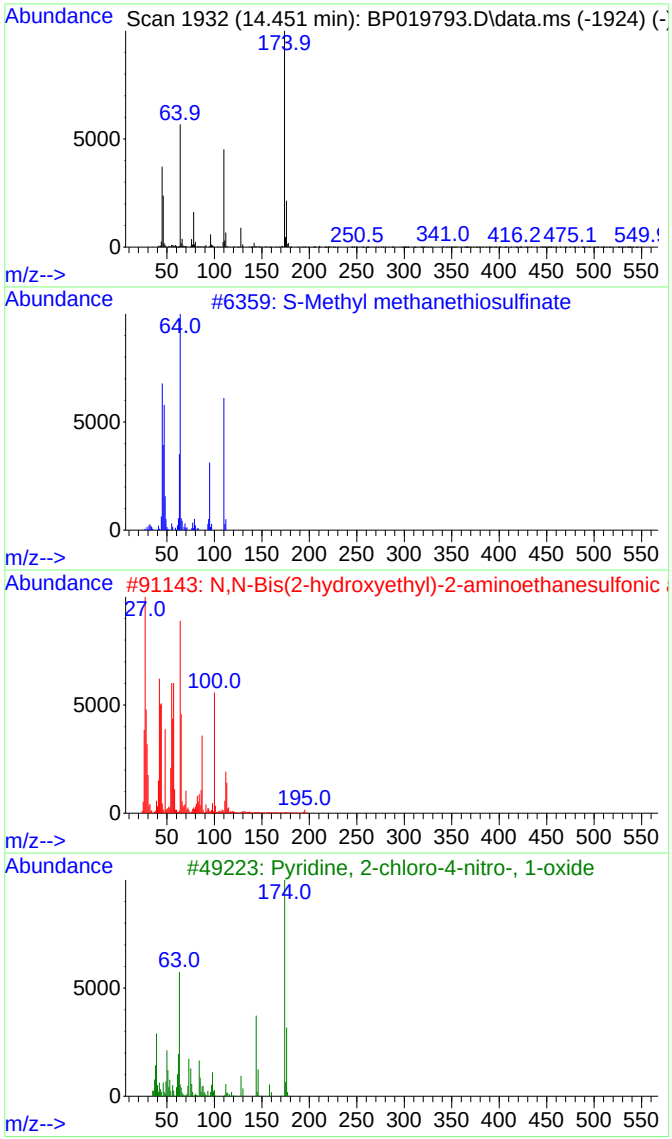
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

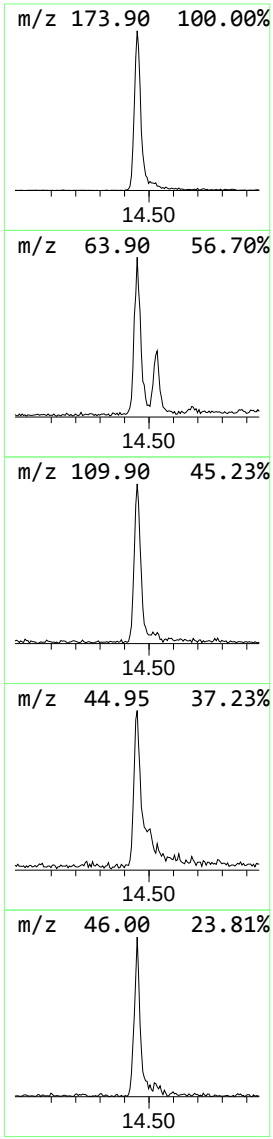
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 S-Methyl methanethiosulfinate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	3.52 ng	138642	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	52
2	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	17
3	Pyridine, 2-chloro-4-nitro-, 1-o...	174	C5H3ClN2O3	014432-16-7	10
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
5	3-Chloro-5-nitro-2(1H)-pyridinone	174	C5H3ClN2O3	022353-38-4	9





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ALS Vial : 18 Sample Multiplier: 1

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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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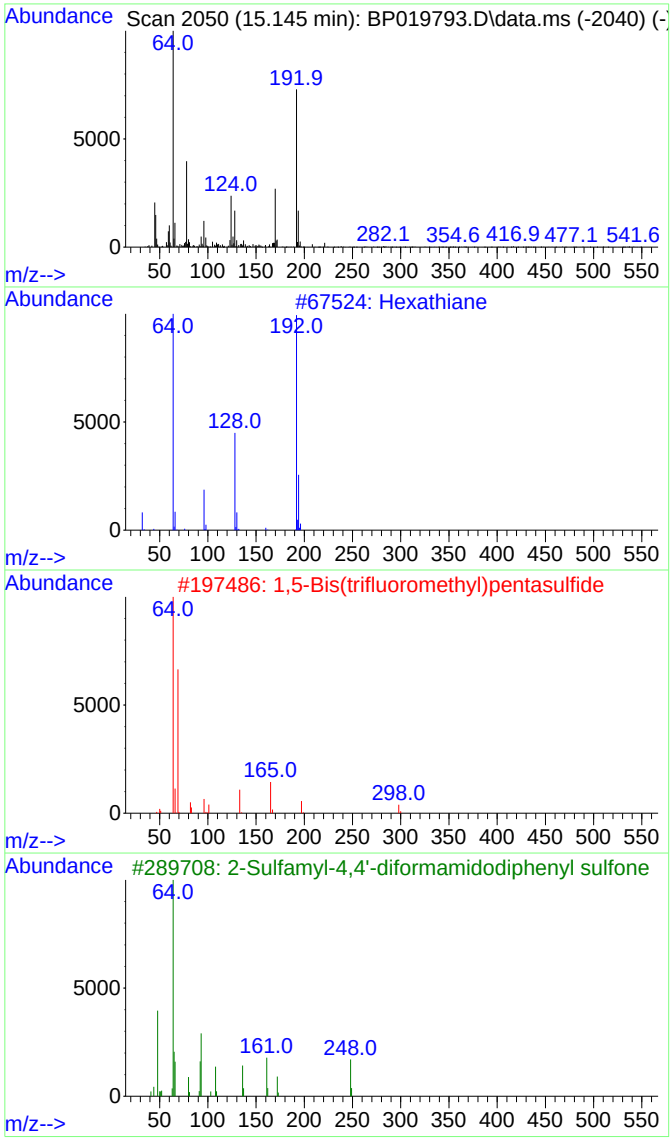
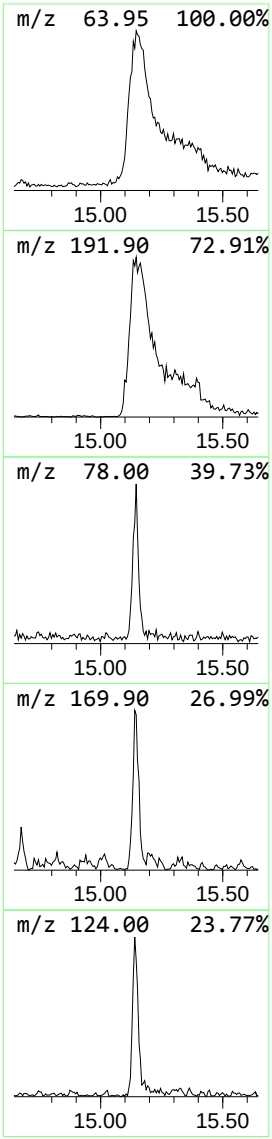
Peak Number 17 Hexathiane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	4.40 ng	173248	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	74
2	1,5-Bis(trifluoromethyl)pentasul...	298	C2F6S5	156412-87-2	36
3	2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	33
4	Butylthiophosphonamidic acid, S-...	167	C5H14NOPS	1000306-05-3	9
5	.alpha.-[9H-Purine-6-thiol-9-yl]...	321	C12H11N5O2S2	019271-00-2	9





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Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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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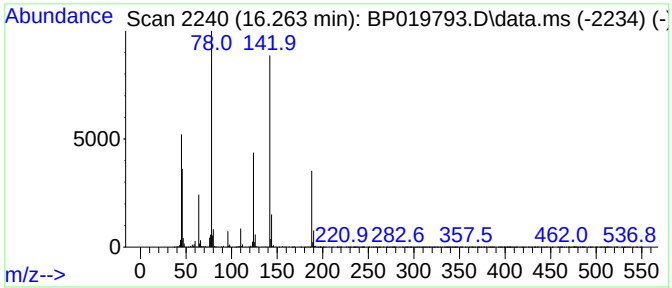
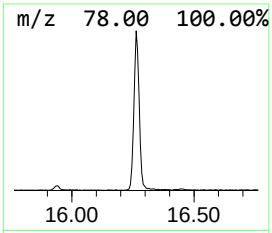
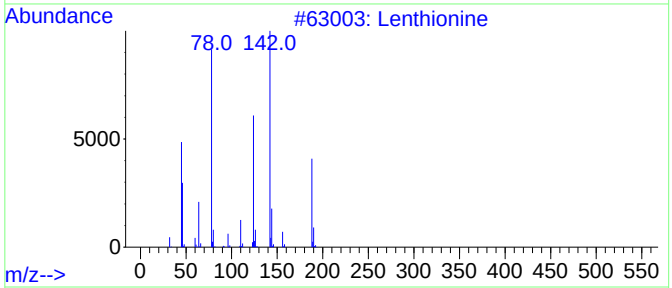
Peak Number 18 Lenthionine Concentration Rank 6

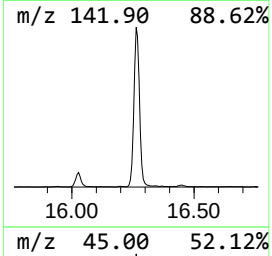
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.263	10.78 ng	585018	Phenanthrene-d10	17.286

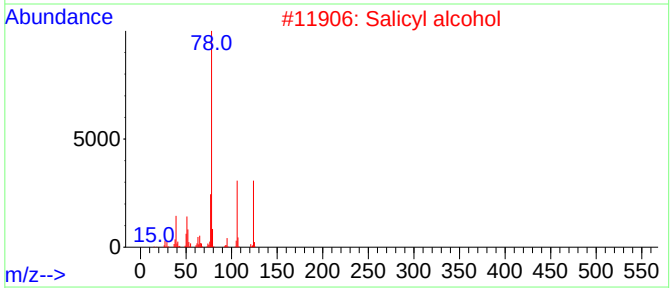
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	86
2	Salicyl alcohol	124	C7H8O2	000090-01-7	50
3	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
4	Cyclohexene, 3-trifluoroacetamid...	305	C10H9F6NO3	1000153-70-3	25
5	Hexathiepane	206	CH2S6	017233-71-5	12

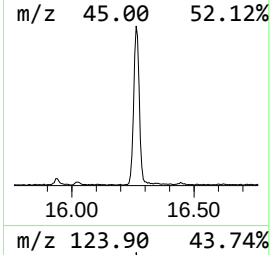


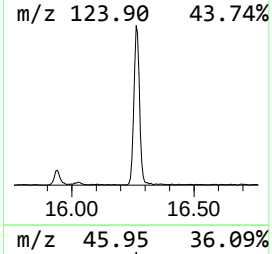


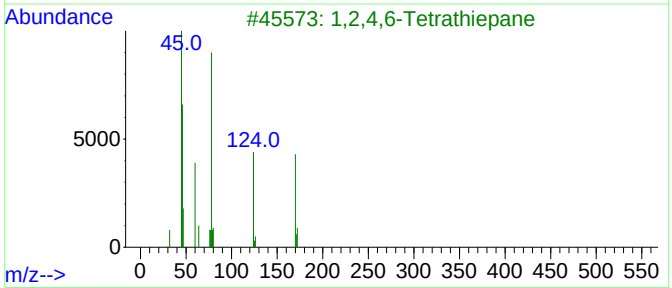


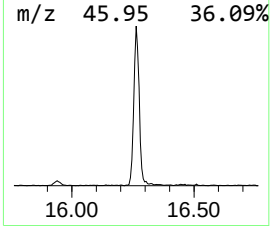












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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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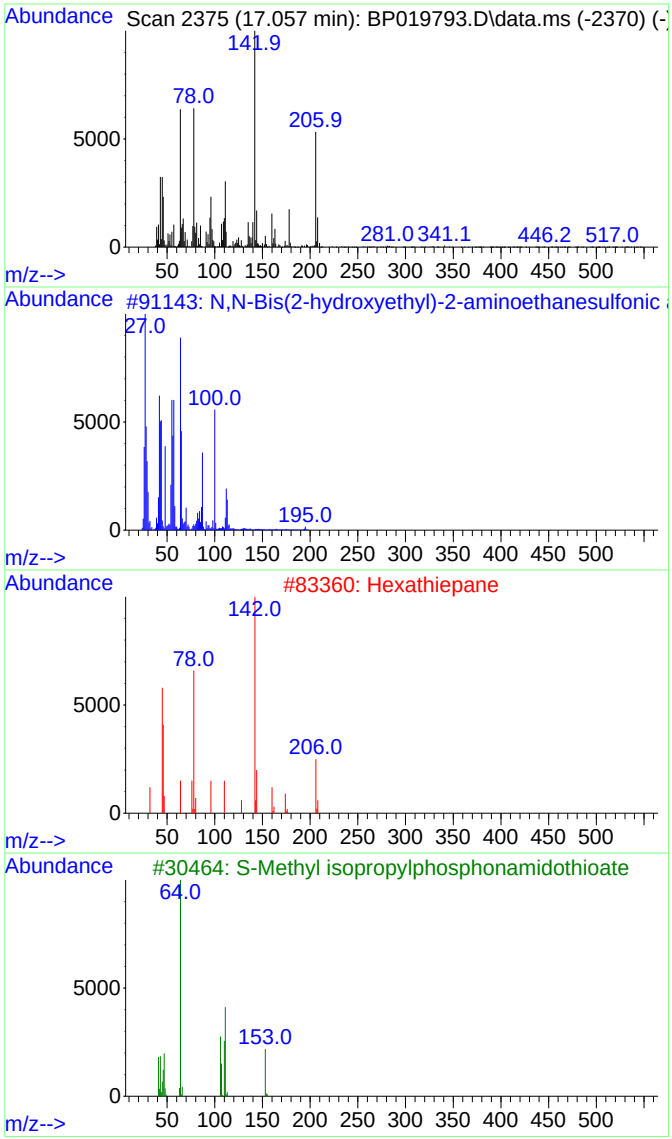
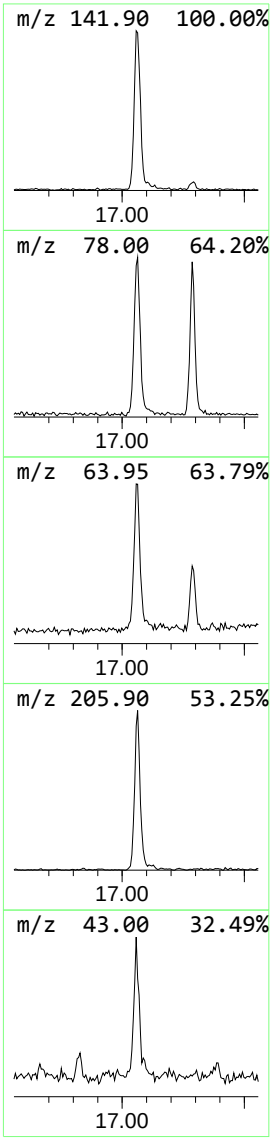
Peak Number 19 unknown17.057 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	4.29 ng	232874	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	27
2	Hexathiepane	206	CH2S6	017233-71-5	25
3	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	17
4	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	16
5	S-2-[3-Succinimidopropylamino]et...	296	C9H16N2O5S2	031701-75-4	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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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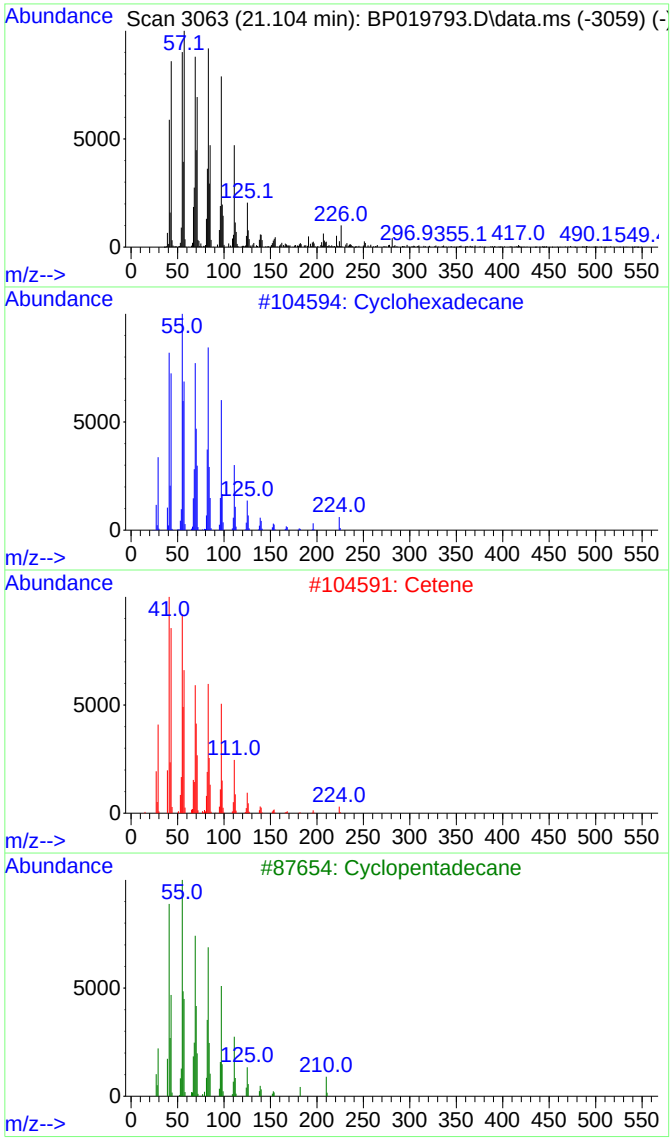
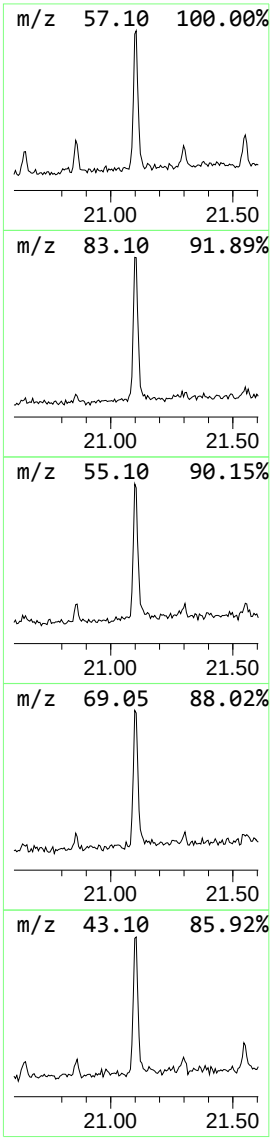
Peak Number 20 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	5.06 ng	316162	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	Cetene	224	C16H32	000629-73-2	96
3	Cyclopentadecane	210	C15H30	000295-48-7	94
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019793.D
Acq On : 20 Feb 2024 19:18
Operator : MA/JU
Sample : P1523-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240766-AMENDED-COMP-39N-N-3-01

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	3.128	120.3	ng	2240340	1	7.893	372389	20.0
2-Butenal, 2-me...	3.746	2.9	ng	53907	1	7.893	372389	20.0
Prenol	4.069	12.3	ng	228723	1	7.893	372389	20.0
Furan, 2,3-dihy...	4.246	3.6	ng	67217	1	7.893	372389	20.0
unknown4.452	4.452	4.3	ng	80744	1	7.893	372389	20.0
2-Pentanol, 4-m...	4.640	16.3	ng	302784	1	7.893	372389	20.0
unknown4.693	4.693	10.7	ng	199775	1	7.893	372389	20.0
2-Pentanone, 4-...	5.016	62.3	ng	1160070	1	7.893	372389	20.0
unknown6.099	6.099	2.7	ng	50448	1	7.893	372389	20.0
unknown6.722	6.722	3.3	ng	61100	1	7.893	372389	20.0
unknown7.593	7.593	4.0	ng	73504	1	7.893	372389	20.0
2(5H)-Furanone,...	8.140	2.8	ng	51145	1	7.893	372389	20.0
unknown8.869	8.869	4.0	ng	75001	1	7.893	372389	20.0
1,2,4,6-Tetrath...	9.428	59.3	ng	1593210	2	10.698	537783	20.0
1,2,4,5-Tetrath...	13.298	4.9	ng	194501	3	14.534	786714	20.0
S-Methyl methan...	14.451	3.5	ng	138642	3	14.534	786714	20.0
Hexathiane	15.145	4.4	ng	173248	3	14.534	786714	20.0
Lenthionine	16.263	10.8	ng	585018	4	17.286	1085270	20.0
unknown17.057	17.057	4.3	ng	232874	4	17.286	1085270	20.0
Cyclohexadecane	21.104	5.1	ng	316162	5	21.380	1249940	20.0