LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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: BP019794.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	18	rVB	1872997	2173185	62.30%	10.154%
2	3.746	108	112	125	rBV3	29022	57926	1.66%	0.271%
3	4.070	160	167	177	rBV	131937	215123	6.17%	1.005%
4	4.246	191	197	202	rBV	41489	60900	1.75%	0.285%
5	4.305	202	207	219	rVV	38710	66745	1.91%	0.312%
6	4.452	228	232	241	rVB	51829	74524	2.14%	0.348%
7	4.640	259	264	269	rVV	198910	289869	8.31%	1.354%
8	4.693	269	273	286	rVB	121683	198876	5.70%	0.929%
9	5.017	322	328	338	rBV	996504	1430652	41.01%	6.684%
10	5.469	397	405	414	rBV	469654	729043	20.90%	3.406%
11	5.793	454	460	465	rBV2	27894	46707	1.34%	0.218%
12	6.099	505	512	516	rBV3	20816	49938	1.43%	0.233%
13	6.211	527	531	537	rVB4	18471	36834	1.06%	0.172%
14	6.722	614	618	625	rBV6	23046	56510	1.62%	0.264%
15	7.069	669	677	684	rBV	538172	905480	25.96%	4.231%
16	7.593	760	766	774	rBV2	39855	71128	2.04%	0.332%
17	7.893	811	817	824	rVB	230215	368704	10.57%	1.723%
18	8.140	852	859	863	rBV3	25885	46315	1.33%	0.216%
19	8.863	977	982	987	rBV3	26891	58658	1.68%	0.274%
20	9.063	1008	1016	1027	rBV	452058	801305	22.97%	3.744%
21	9.358	1057	1066	1070	rBV8	17661	48423	1.39%	0.226%
22	9.428	1070	1078	1088	rVV	742625	1368263	39.22%	6.393%
23	9.510	1089	1092	1107	rVB10	15298	39888	1.14%	0.186%
24	10.052	1180	1184	1198	rBV5	19543	61145	1.75%	0.286%
25	10.699	1285	1294	1309	rBV	273400	506950	14.53%	2.369%
26	11.075	1352	1358	1364	rBV5	20026	51662	1.48%	0.241%
27	11.452	1416	1422	1429	rBV4	26300	52238	1.50%	0.244%
28	13.157	1701	1712	1723	rBV	1129183	1788448	51.27%	8.356%
29	13.298	1731	1736	1743	rVB	89364	151308	4.34%	0.707%
30	13.587	1777	1785	1792	rBV2	39396	74028	2.12%	0.346%
31	14.451	1925	1932	1939	rBV	45775	93584	2.68%	0.437%
32	14.528	1939	1945	1956	rVV	406751	670833	19.23%	3.134%
33	15.140	2040	2049	2064	rBV3	29384	98725	2.83%	0.461%
34	16.028	2193	2200	2208	rBV	479007	752011	21.56%	3.514%
35	16.263	2234	2240	2253	rVB	209996	352333	10.10%	1.646%
36	17.063	2370	2376	2388	rVB2	103365	186998	5.36%	0.874%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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	17.287	2408	2414	2428	rBV	589796	938167	26.89%	4.383%
38	18.181	2562	2566	2573	rBV	75192	111445	3.19%	0.521%
39	19.298	2753	2756	2761	rVB	32347	44911	1.29%	0.210%
40	19.422	2773	2777	2780	rBV5	26177	38417	1.10%	0.179%
41	19.616	2806	2810	2813	rBV2	61940	87902	2.52%	0.411%
42	19.851	2845	2850	2860	rBV	2724209	3488270	100.00%	16.298%
43	20.863	3019	3022	3025	rVB	37923	41999	1.20%	0.196%
44	21.098	3059	3062	3068	rVB	180449	235264	6.74%	1.099%
45	21.380	3105	3110	3121	rBV	827933	1201919	34.46%	5.616%
46	23.798	3514	3521	3532	rVB	521944	1179692	33.82%	5.512%

Sum of corrected areas: 21403245

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
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Instrument :
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ClientSampleId :
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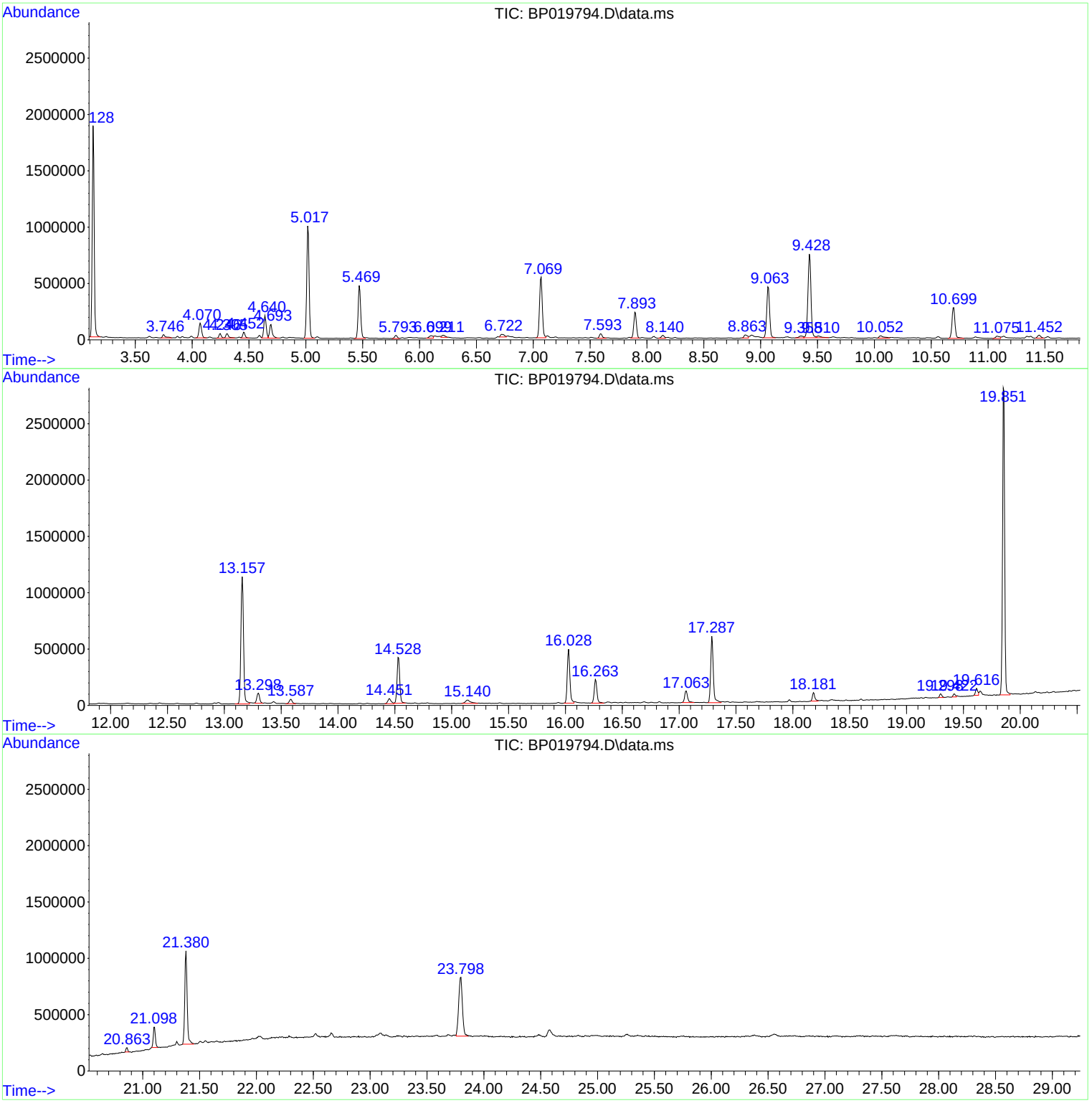
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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

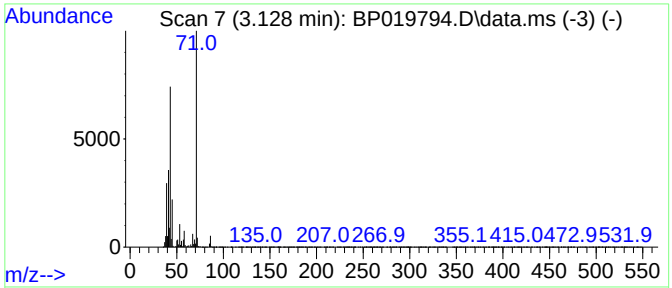
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

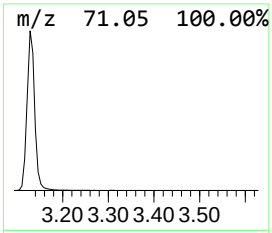
****

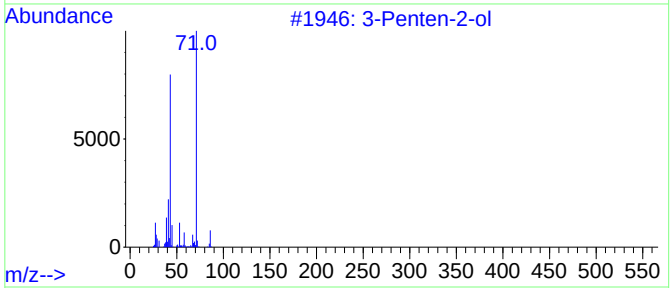
Peak Number 1 3-Penten-2-ol Concentration Rank 1

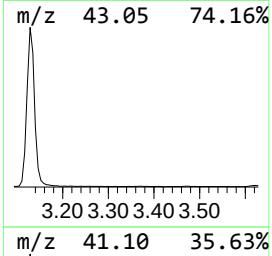
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	117.88 ng	2173190	1,4-Dichlorobenzene-d4	7.893

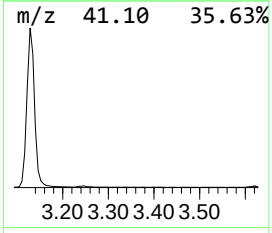
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	80
2	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	50
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50
5	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	45

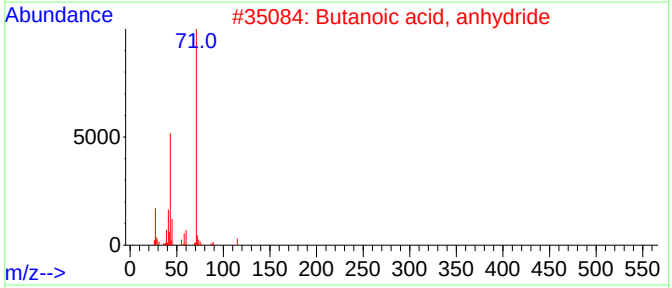


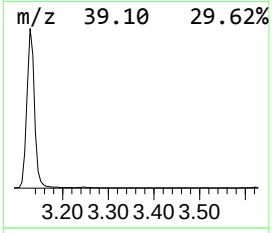


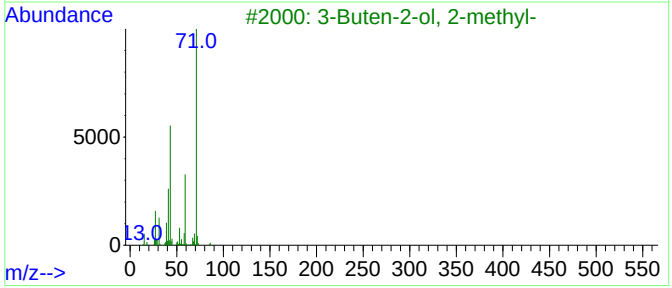


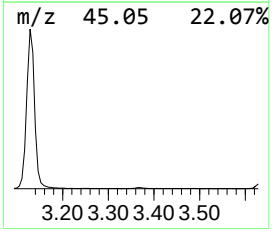












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Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

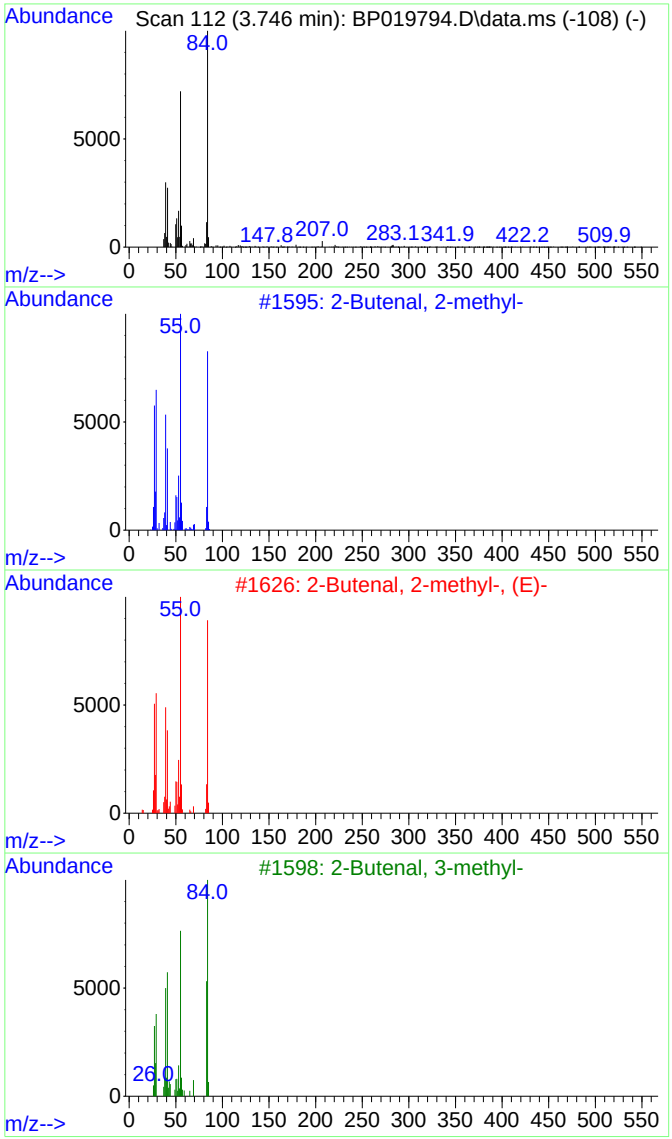
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

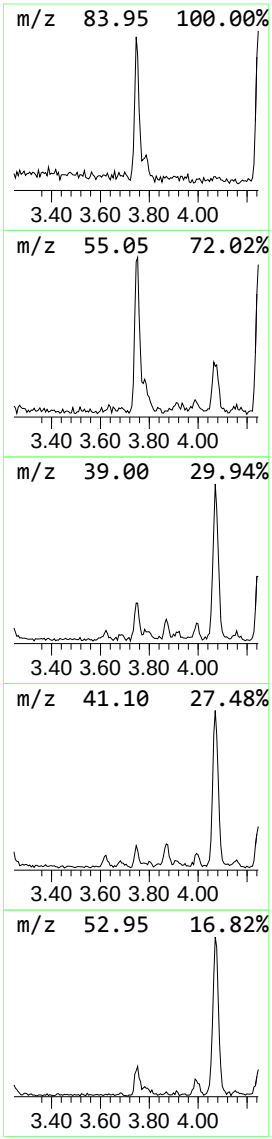
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butenal, 2-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.746	3.14 ng	57926	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	90
2	2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	90
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	78
4	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	58
5	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
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Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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

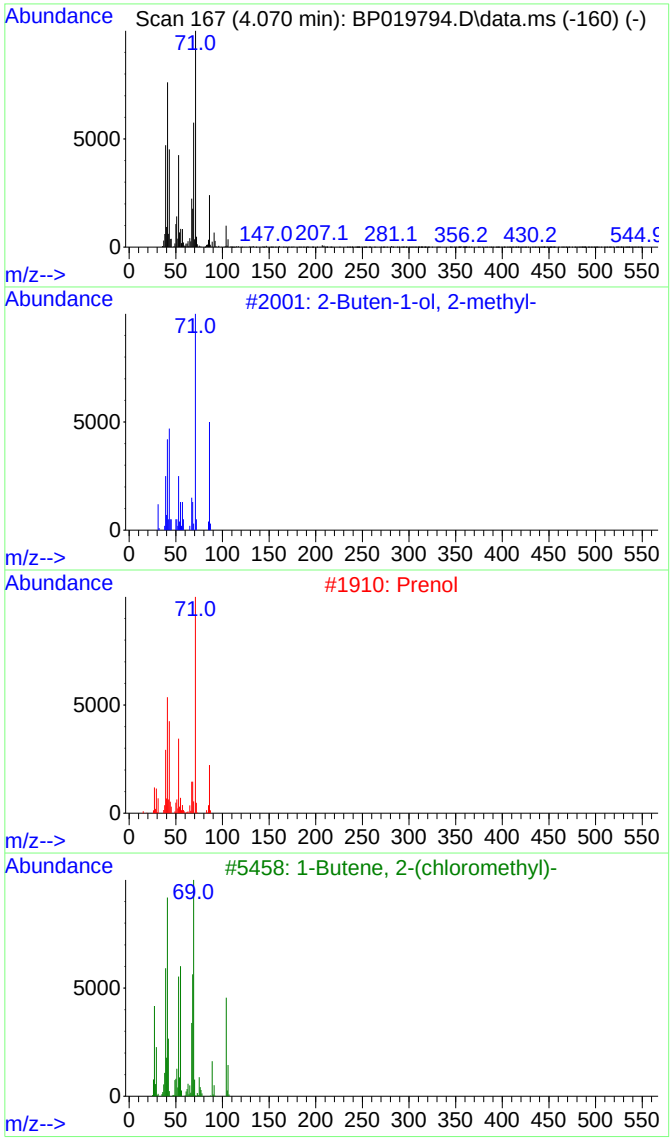
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

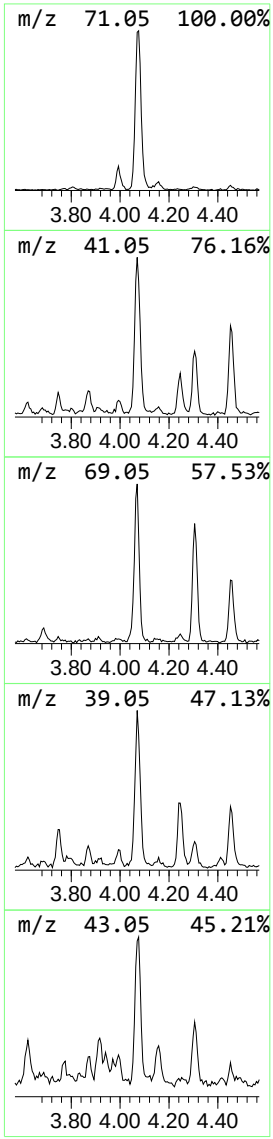
****

Peak Number 3 2-Buten-1-ol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.070	11.67 ng	215123	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	74
2	Prenol	86	C5H10O	000556-82-1	72
3	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	53
4	1-Butene, 1-chloro-3-methyl-	104	C5H9Cl	023010-00-6	43
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	27





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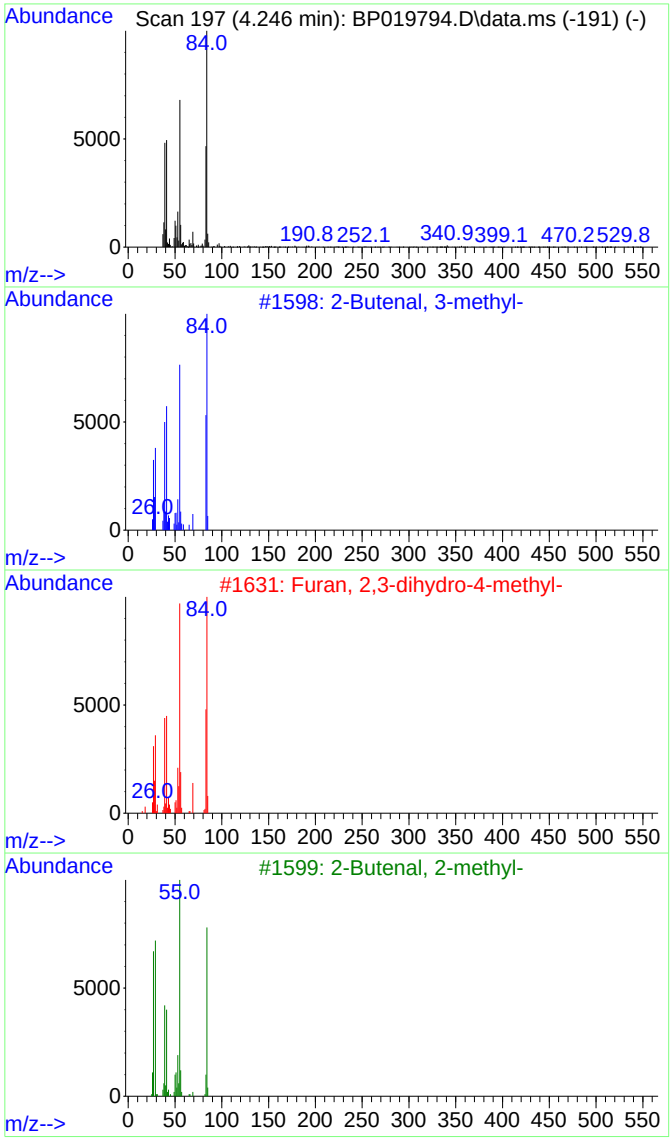
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

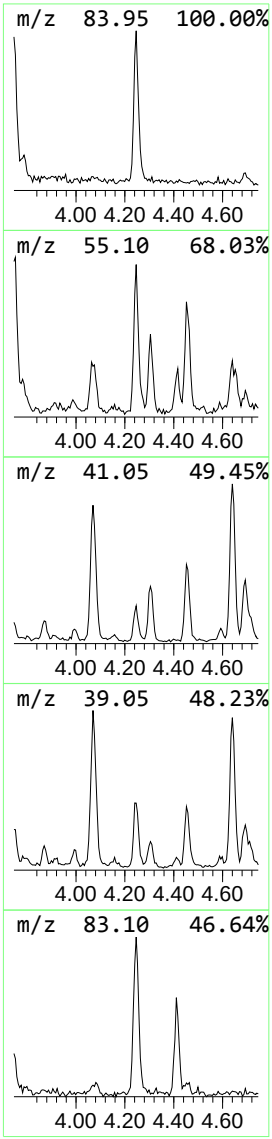
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butenal, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.246	3.30 ng	60900	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	94
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	72
3	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	68
4	Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	64
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	50





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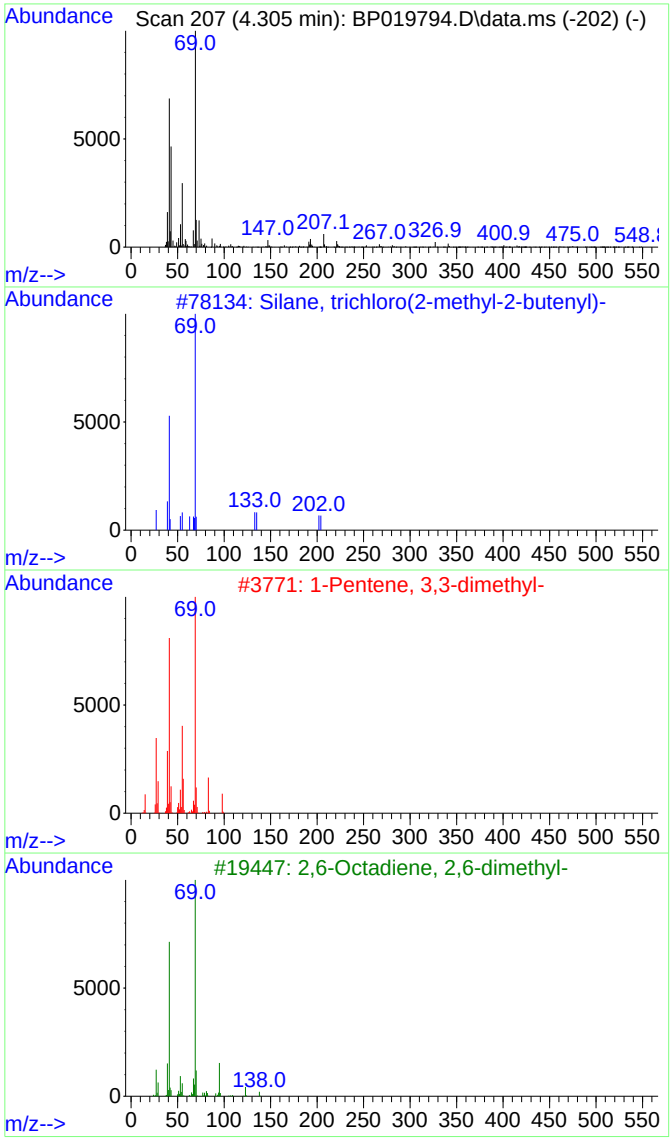
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

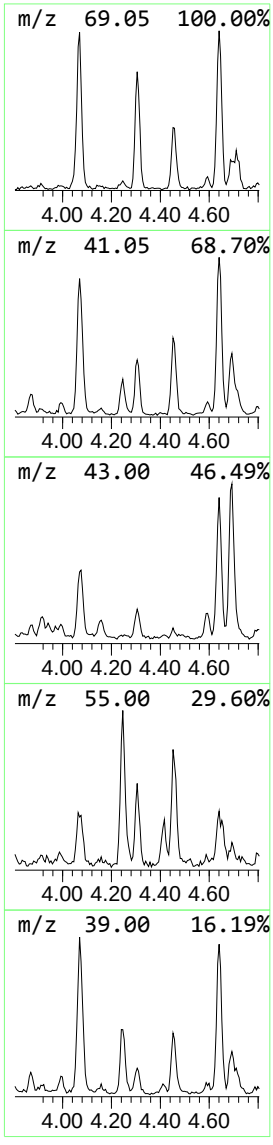
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Silane, trichloro(2-methyl-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.305	3.62 ng	66745	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, trichloro(2-methyl-2-but...	202	C5H9Cl3Si	018163-57-0	53
2	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	42
3	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	42
4	1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	42
5	4-Trifluoroacetoxyoctane	226	C10H17F3O2	116465-17-9	42





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

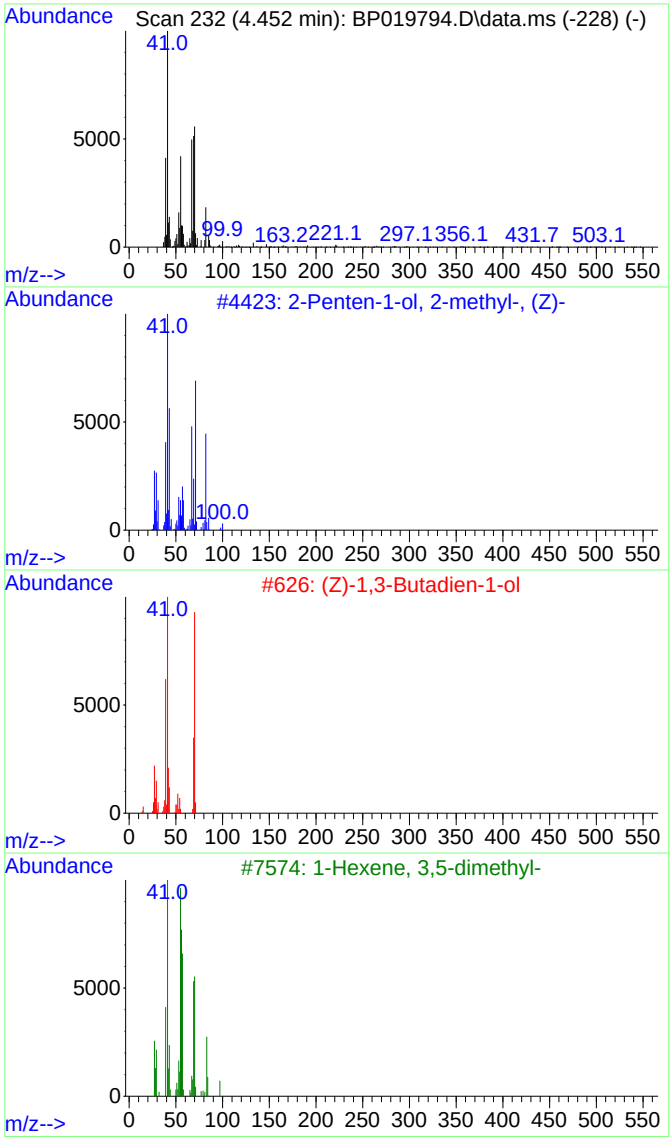
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

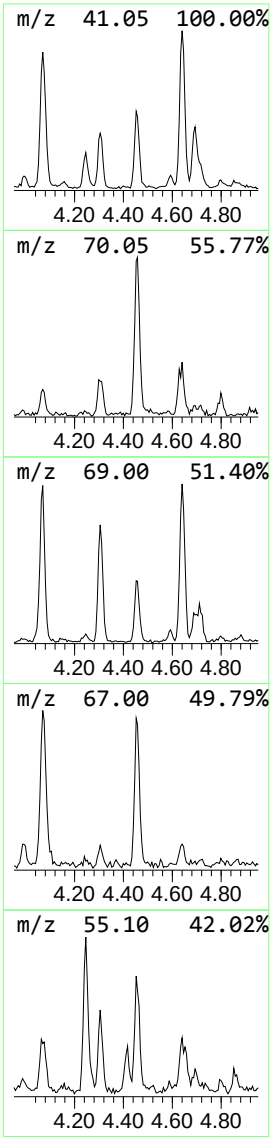
****

Peak Number 6 unknown4.452 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	4.04 ng	74524	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Penten-1-ol, 2-methyl-, (Z)-	100	C6H12O	016958-20-6	43
2	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	38
3	1-Hexene, 3,5-dimethyl-	112	C8H16	007423-69-0	37
4	2-Butenenitrile	67	C4H5N	004786-20-3	35
5	3-Hexen-1-ol, (E)-	100	C6H12O	000928-97-2	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

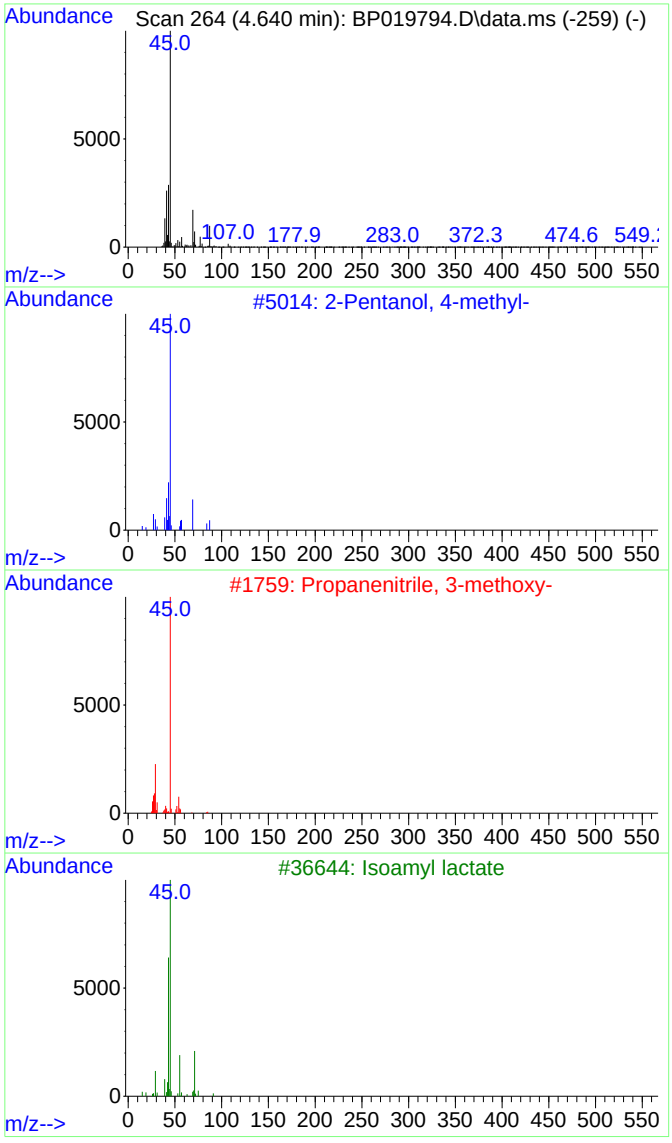
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

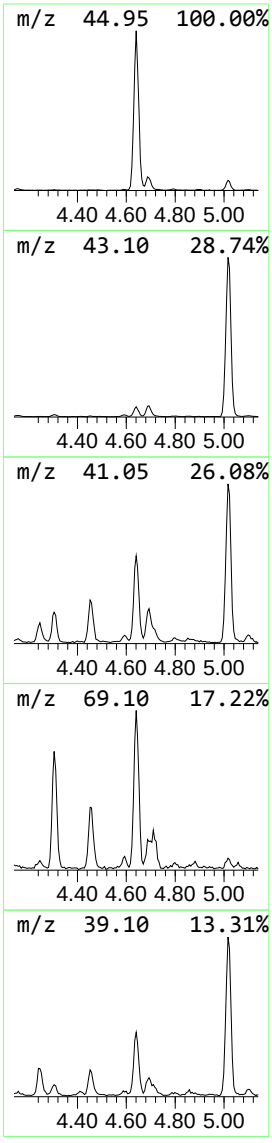
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	15.72 ng	289869	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	50
2	Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	40
3	Isoamyl lactate	160	C8H16O3	019329-89-6	36
4	4-Penten-2-ol	86	C5H10O	000625-31-0	36
5	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	33





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Sample : P1523-07
Misc :
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ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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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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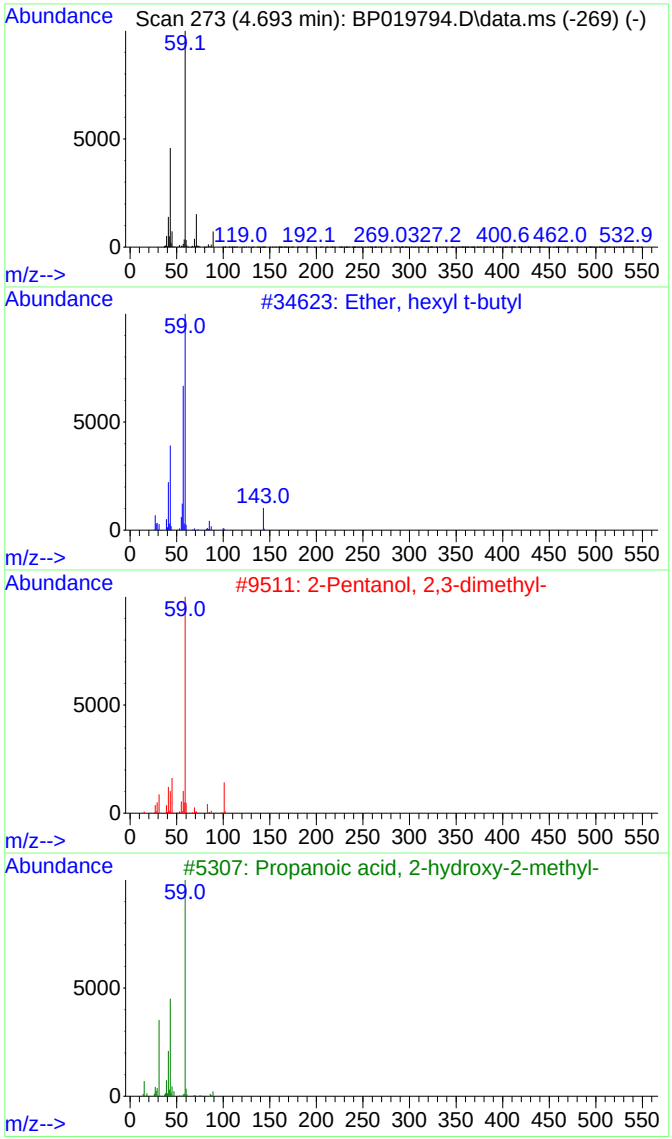
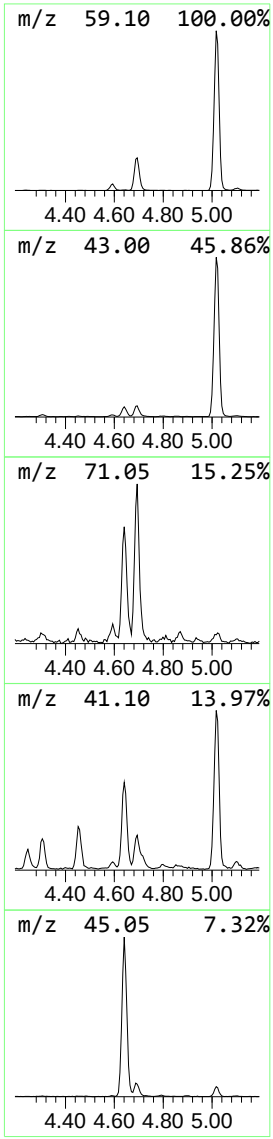
Peak Number 8 unknown4.693 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.693	10.79 ng	198876	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	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	45
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	42
4	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	39
5	Tri(propylene glycol) propyl ether	234	C12H26O4	096077-04-2	38





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Sample : P1523-07
Misc :
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Instrument :
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ClientSampleId :
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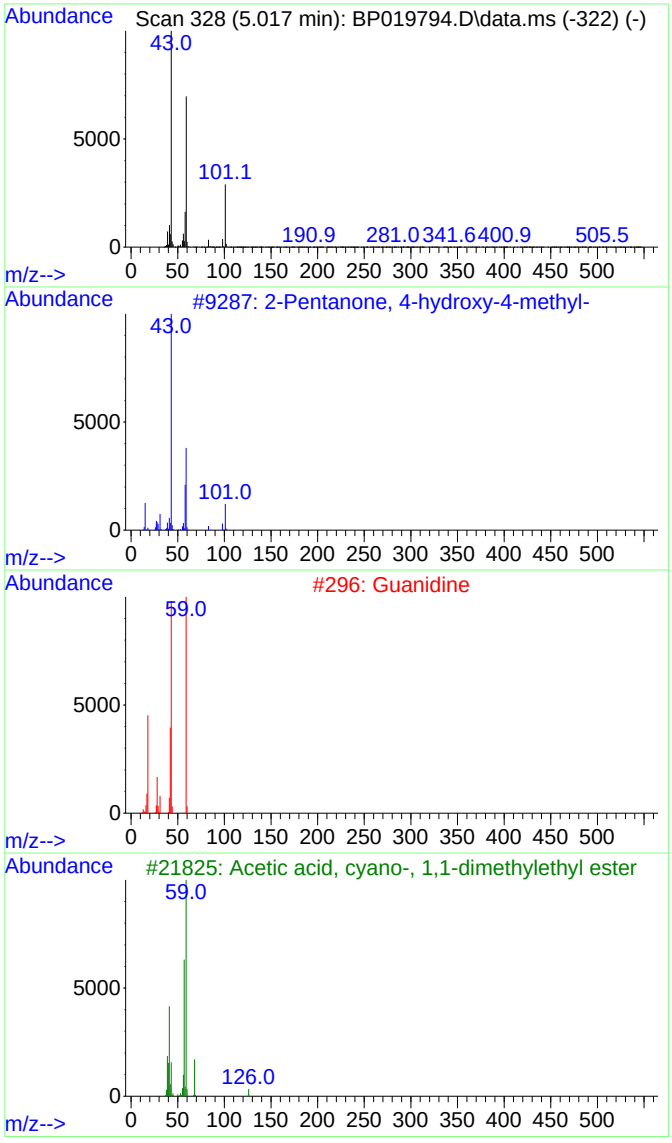
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

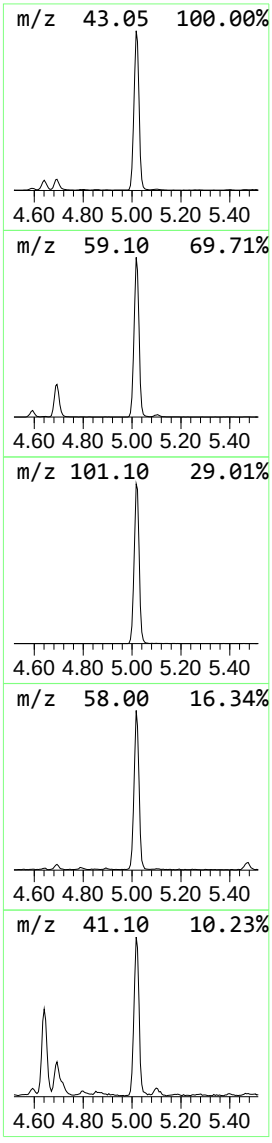
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.017	77.60 ng	1430650	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	64
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	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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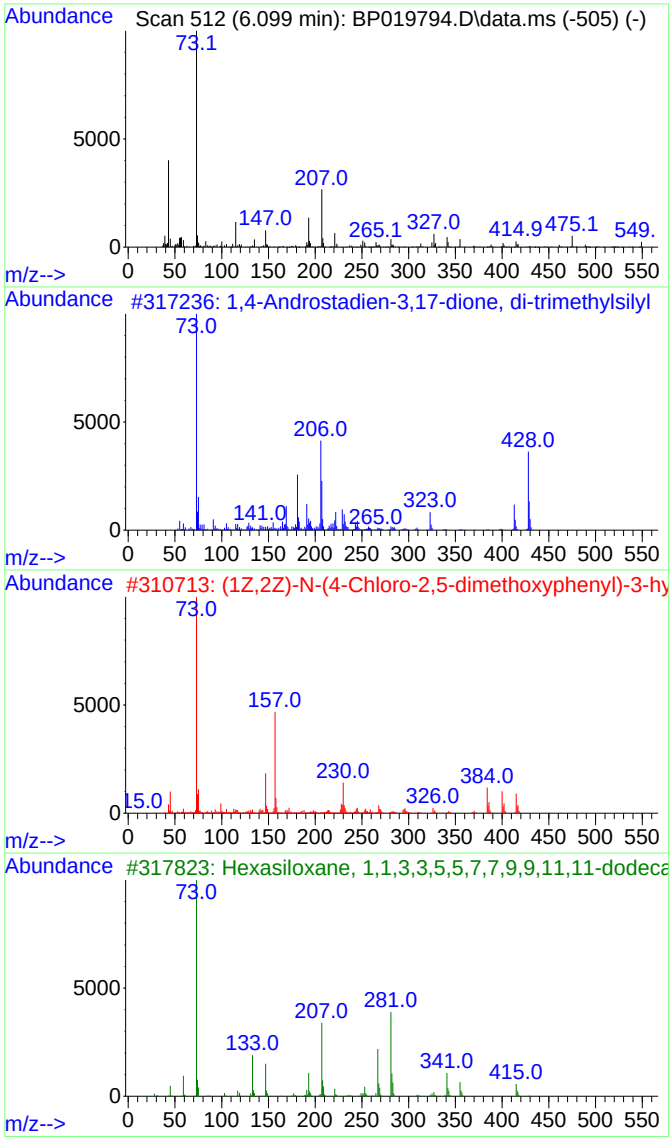
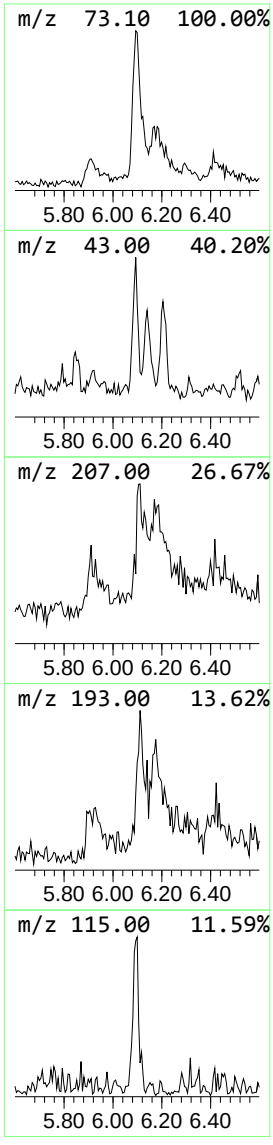
Peak Number 10 unknown6.099 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.099	2.71 ng	49938	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Androstadien-3,17-dione, di-...	428	C25H40O2Si2	1000412-25-4	28
2	(1Z,2Z)-N-(4-Chloro-2,5-dimethox...	415	C18H30ClNO4Si2	1000477-55-9	25
3	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	25
4	2-(5-Bromo-2-hydroxyphenyl)-1,3-...	519	C19H34BrNO3SSi3	1000479-71-2	25
5	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	25





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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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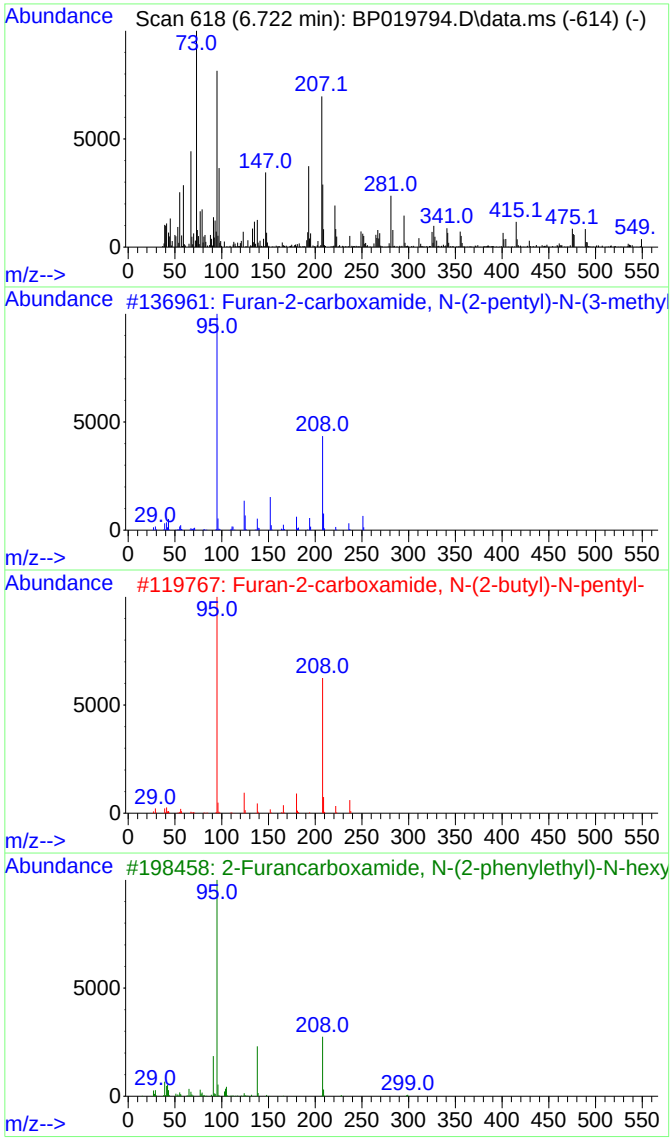
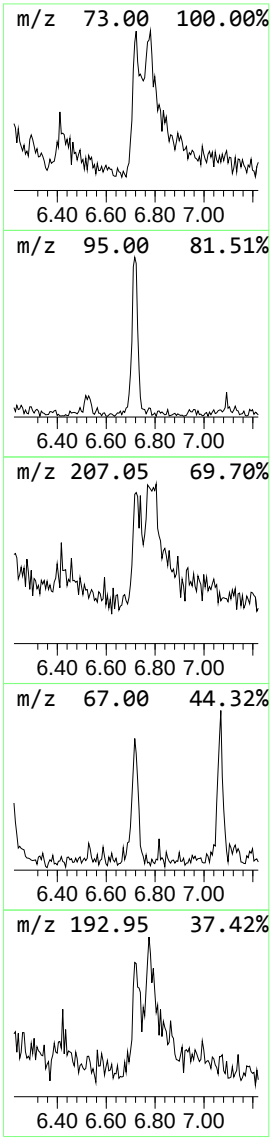
Peak Number 11 unknown6.722 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	3.07 ng	56510	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan-2-carboxamide, N-(2-pentyl...	251	C15H25NO2	1000464-81-0	43
2	Furan-2-carboxamide, N-(2-butyl)...	237	C14H23NO2	1000458-95-9	43
3	2-Furancarboxamide, N-(2-phenyle...	299	C19H25NO2	1000451-27-1	43
4	Furan-2-carboxamide, N-(2-pentyl...	251	C15H25NO2	1000464-81-1	38
5	2-Furancarboxamide, N-[2-(triflu...	295	C13H8F3N3O2	1000320-17-7	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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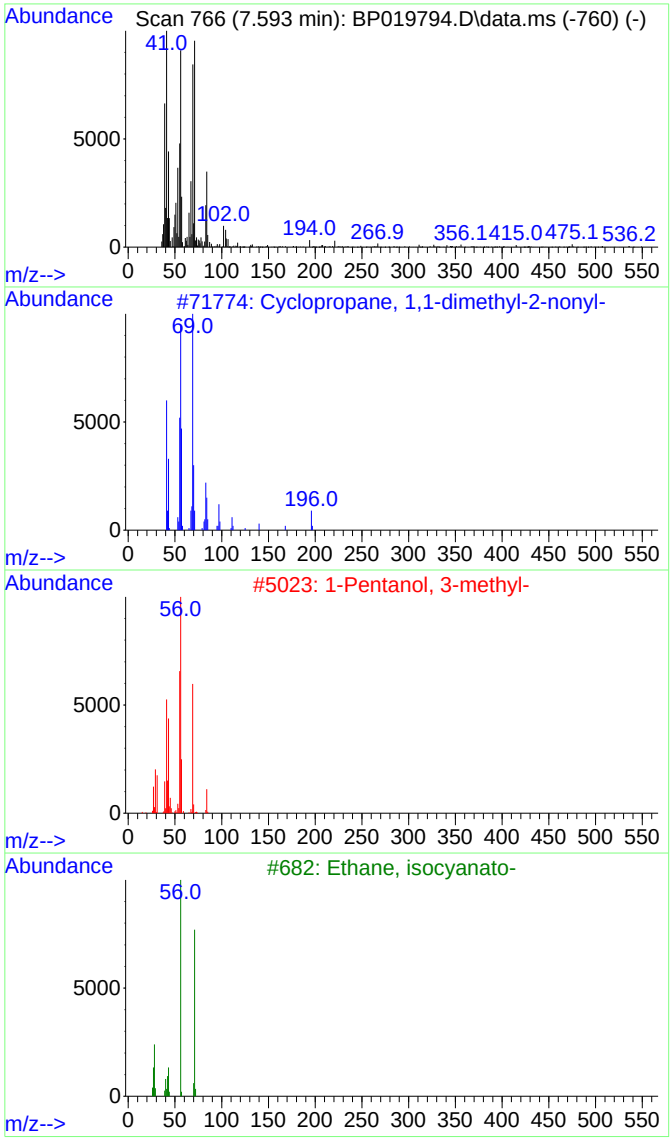
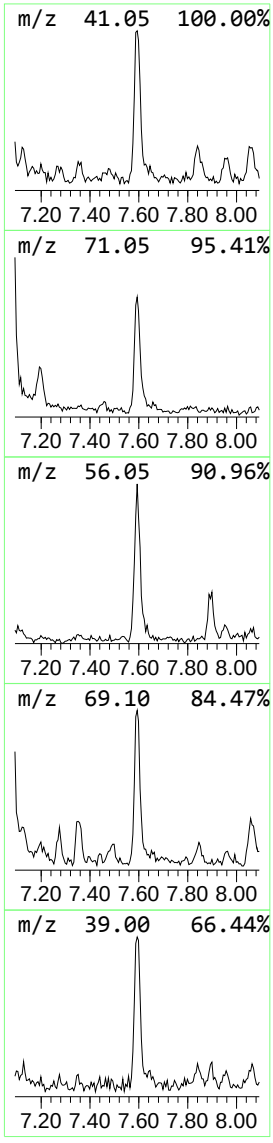
Peak Number 12 unknown7.593 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.593	3.86 ng	71128	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-2-nonyl-	196	C14H28	041977-38-2	47
2	1-Pentanol, 3-methyl-	102	C6H14O	000589-35-5	47
3	Ethane, isocyanato-	71	C3H5NO	000109-90-0	43
4	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	30
5	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	27





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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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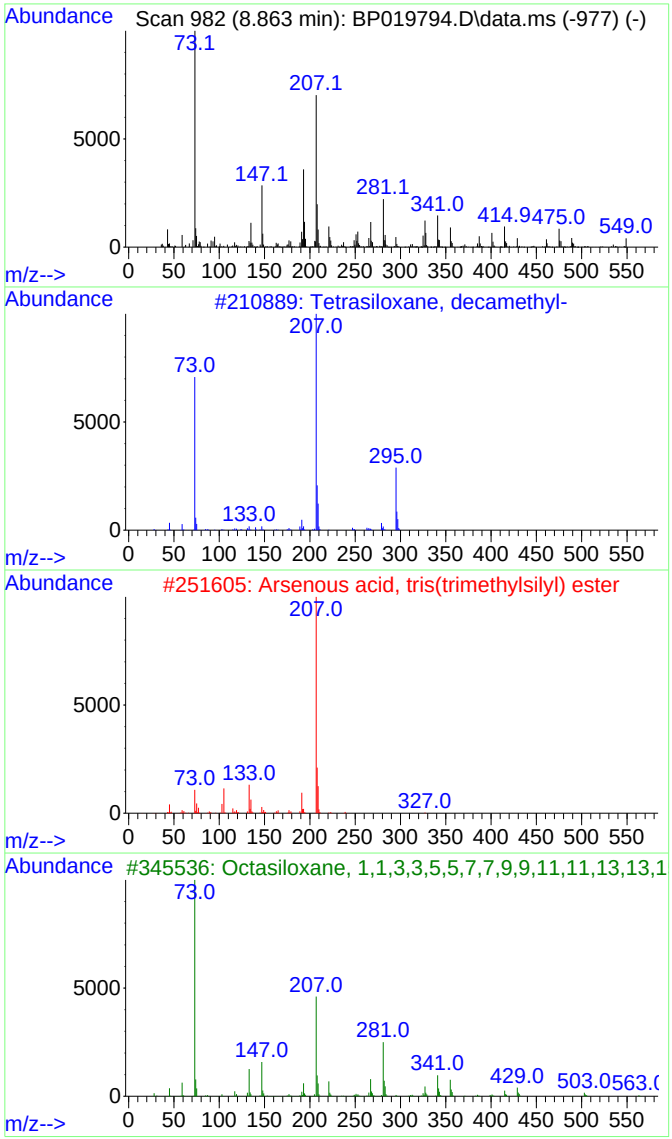
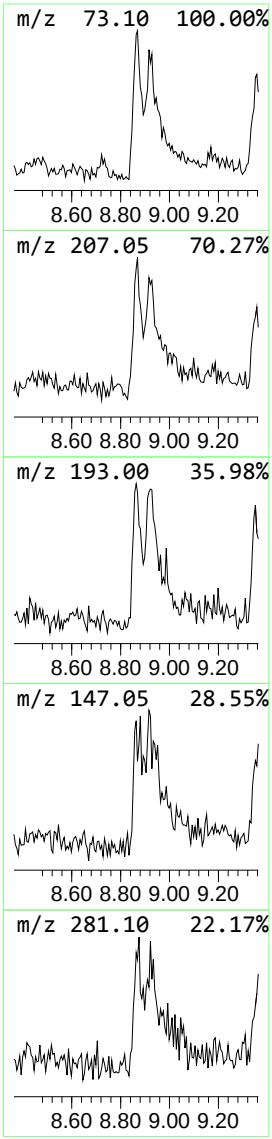
Peak Number 13 unknown8.863 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.863	3.18 ng	58658	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	43
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	38
3	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	38
4	6a-Hydroxy-3,13-dimethoxy-4a,7a,...	488	C26H32O9	1010475-65-9	37
5	2,4-Cyclohexadien-1-one, 3,5-bis...	222	C14H22O2	054965-43-4	32





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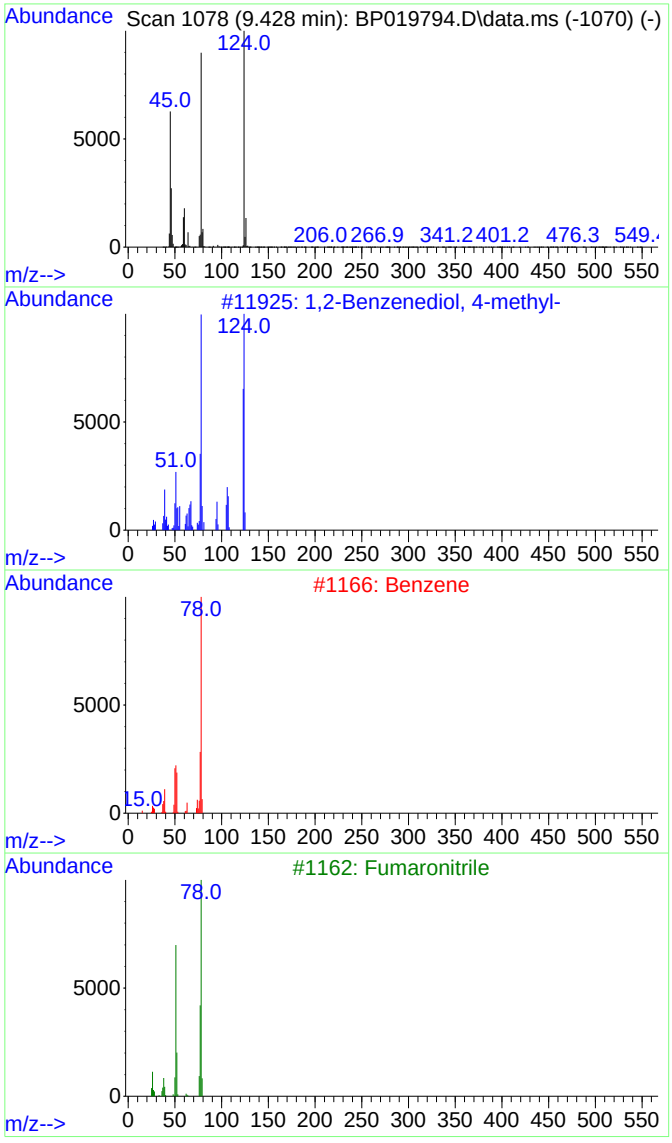
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

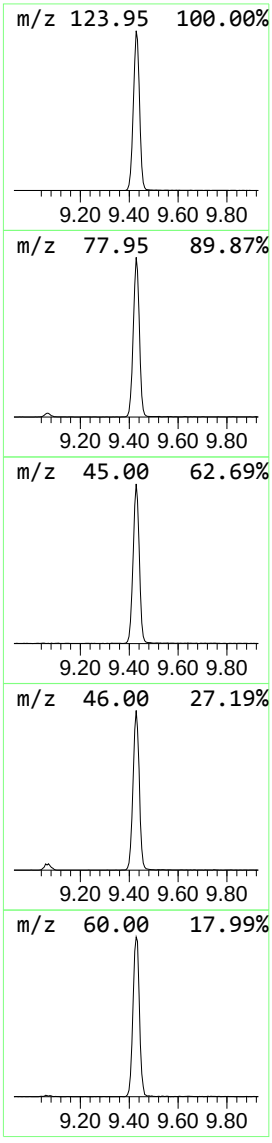
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1,2-Benzenediol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.428	53.98 ng	1368260	Naphthalene-d8	10.699

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2	Benzene	78	C6H6	000071-43-2	9
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	9
5	2,4-Hexadiyne	78	C6H6	002809-69-0	7





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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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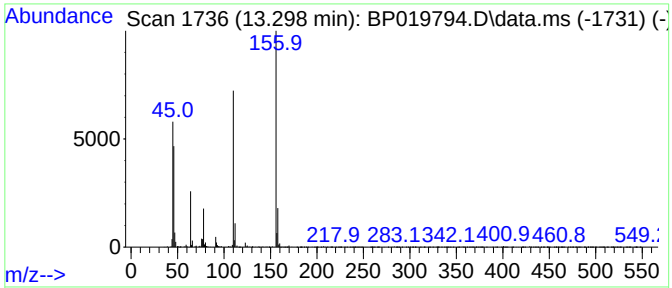
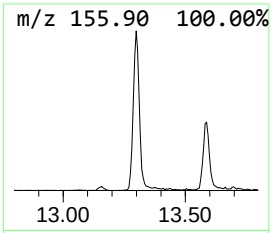
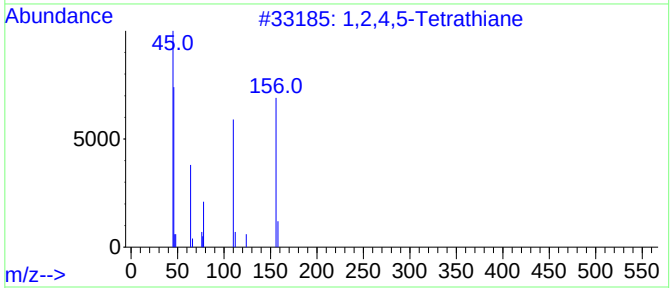
Peak Number 15 unknown13.299 Concentration Rank 8

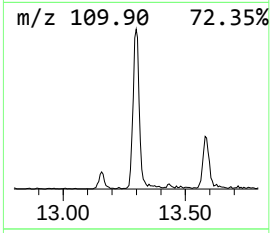
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.299	4.51 ng	151308	Acenaphthene-d10	14.528

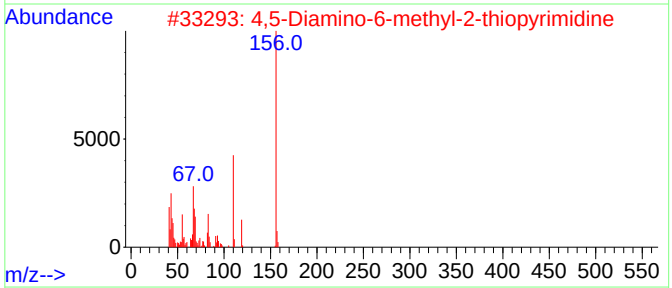
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	40
2	4,5-Diamino-6-methyl-2-thiopyrim...	156	C5H8N4S	006305-99-3	38
3	Omethoate	213	C5H12NO4PS	001113-02-6	25
4	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	25
5	4-Methyl-6-(methylsulfanyl)-1,3,...	156	C5H8N4S	027622-90-8	17

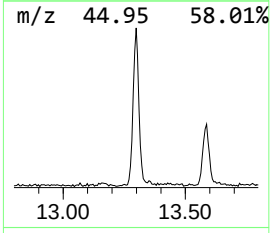


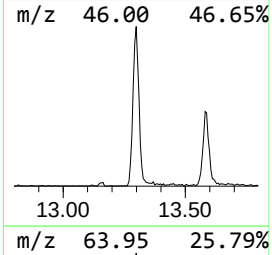


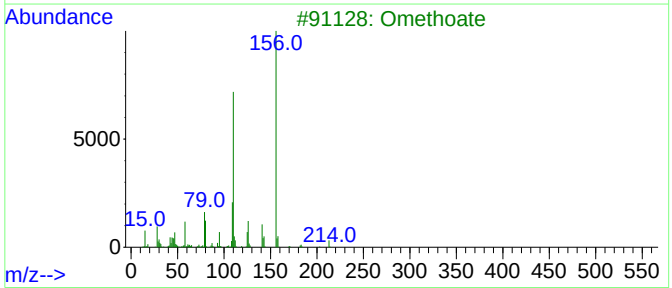


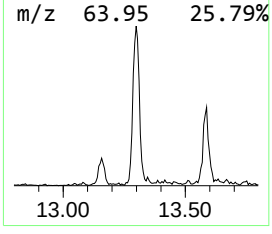












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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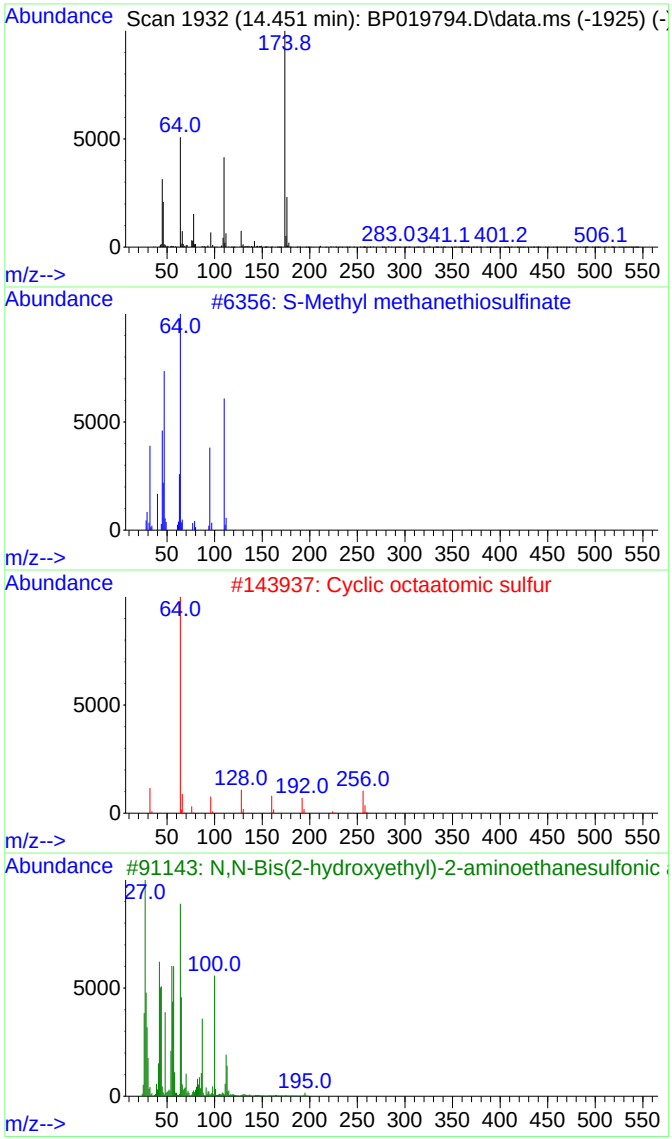
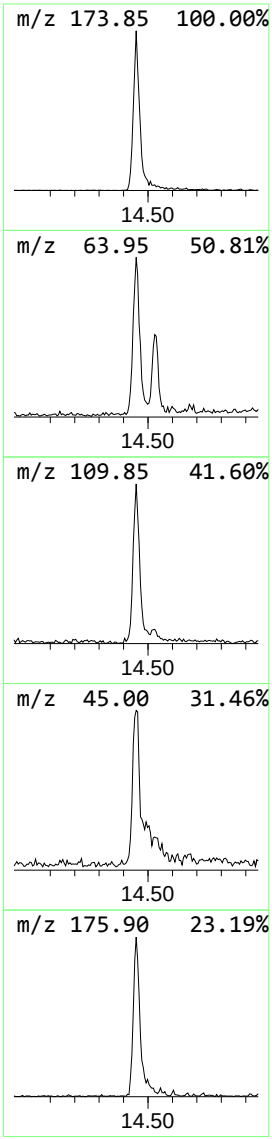
Peak Number 16 unknown14.451 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	2.79 ng	93584	Acenaphthene-d10	14.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	40
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	35
3	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	35
4	Pyridine, 2-chloro-4-nitro-, 1-o...	174	C5H3ClN2O3	014432-16-7	10
5	3-Chloro-5-nitro-2(1H)-pyridinone	174	C5H3ClN2O3	022353-38-4	9





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Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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

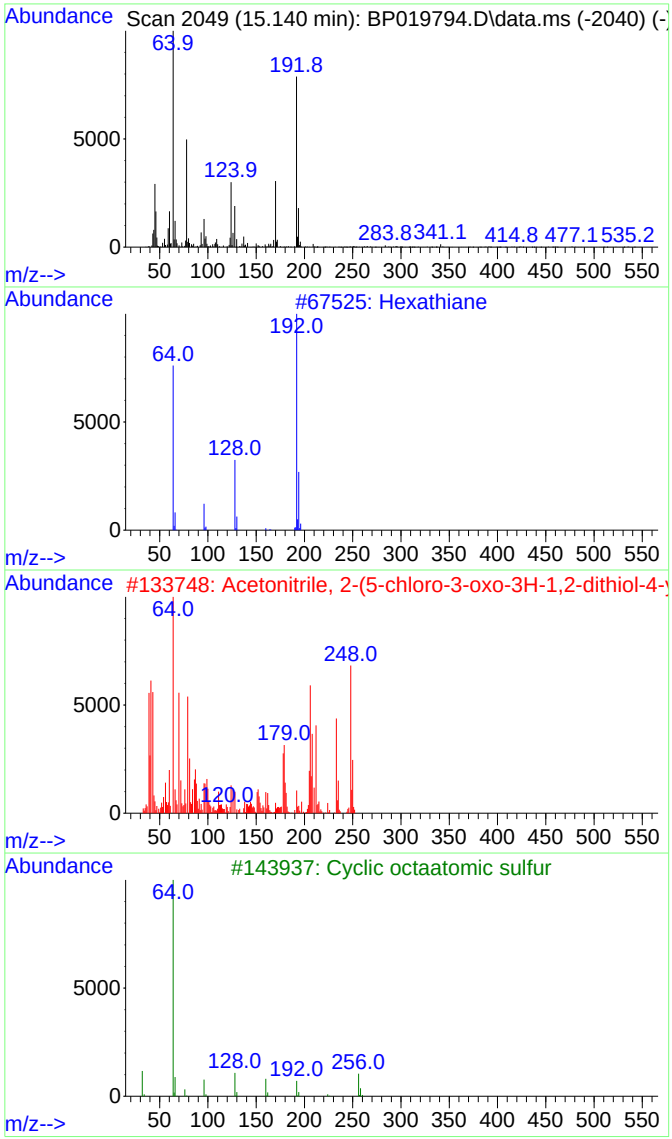
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

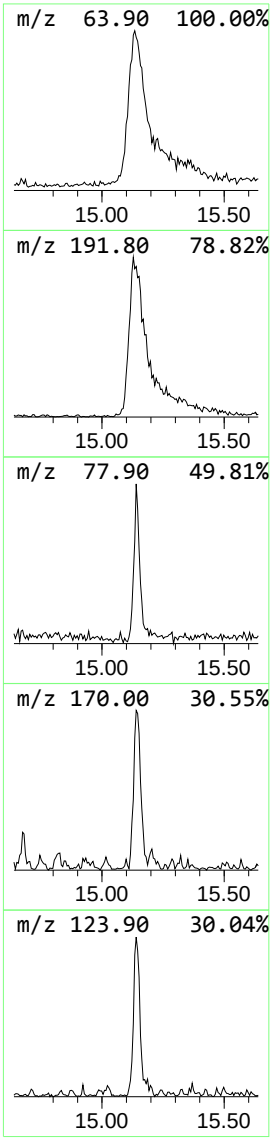
****

Peak Number 17 Hexathiane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.140	2.94 ng	98725	Acenaphthene-d10	14.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	87
2	Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2OS2	1000269-94-4	38
3	Cyclic octaatomic sulfur	256	S8	010544-50-0	33
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	28
5	2,6-Dichloro-4-nitrobenzene-1-su...	289	C6H2Cl3NO4S	074875-17-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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

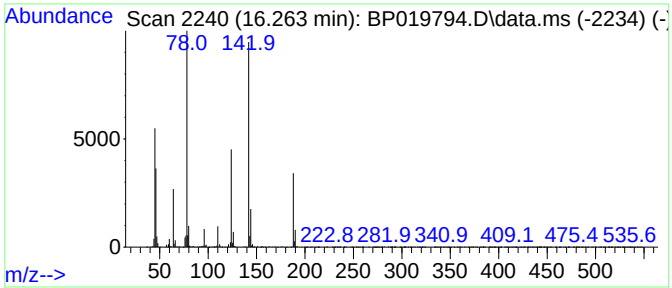
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

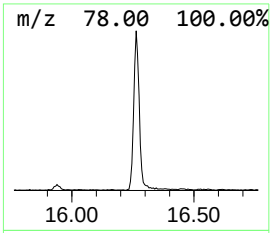
****

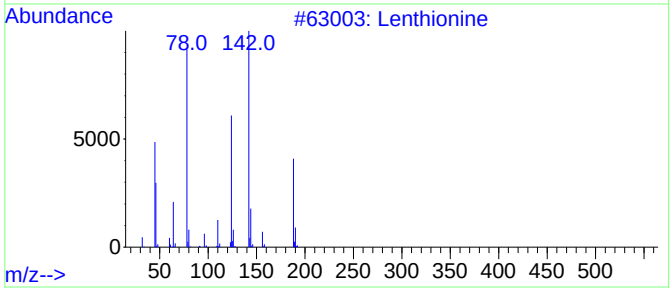
Peak Number 18 Lenthionine Concentration Rank 7

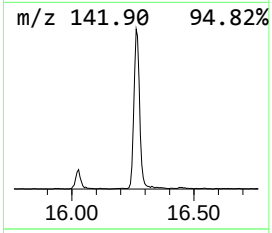
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.263	7.51 ng	352333	Phenanthrene-d10	17.287

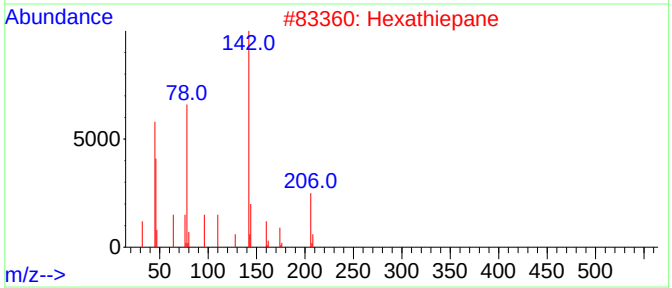
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	97
2	Hexathiepane	206	CH2S6	017233-71-5	38
3	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	38
4	Ehylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	33
5	Cyclohexene, 3-trifluoroacetamid...	305	C10H9F6NO3	1000153-70-3	25

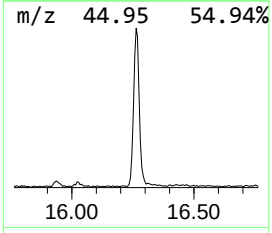


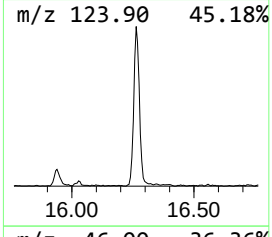


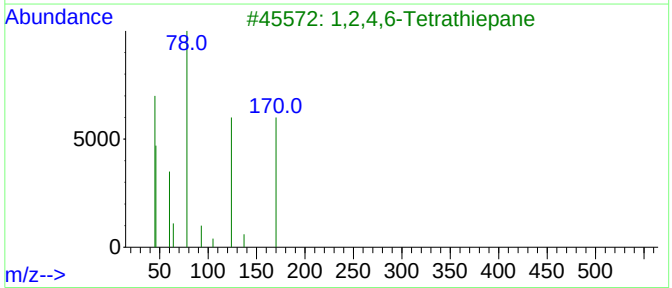


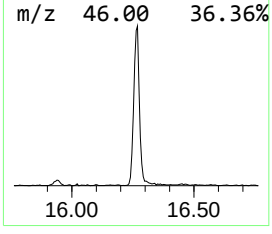












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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

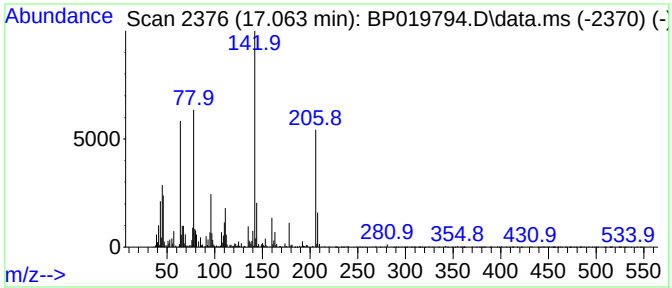
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

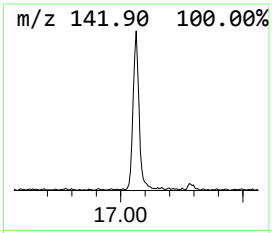
****

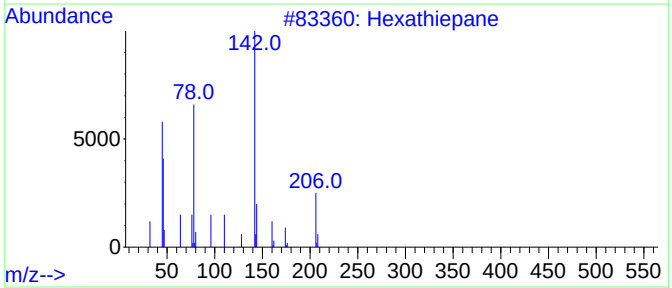
Peak Number 19 unknown17.063 Concentration Rank 10

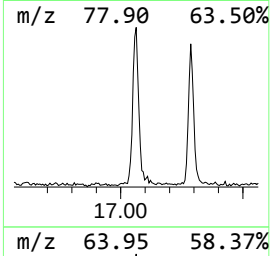
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.063	3.99 ng	186998	Phenanthrene-d10	17.287

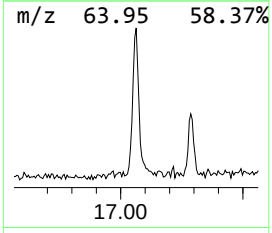
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	17
2	2,6-Dichloro-4-nitrobenzene-1-su...	289	C6H2Cl3NO4S	074875-17-5	12
3	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	12
4	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	12
5	3-Cyclopentylpropionamide, N-(2-...	357	C24H39NO	1000451-37-4	10

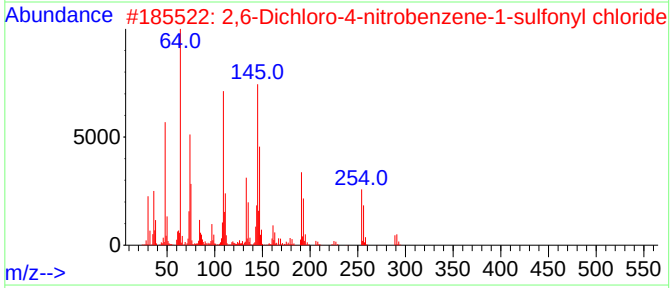


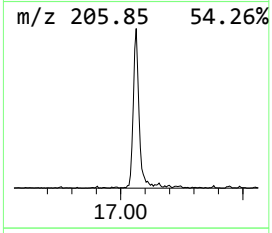


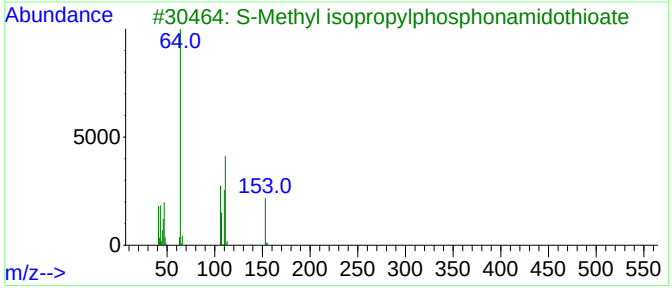


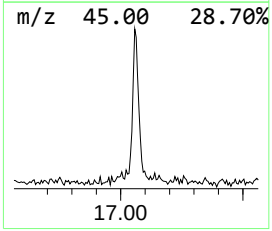












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

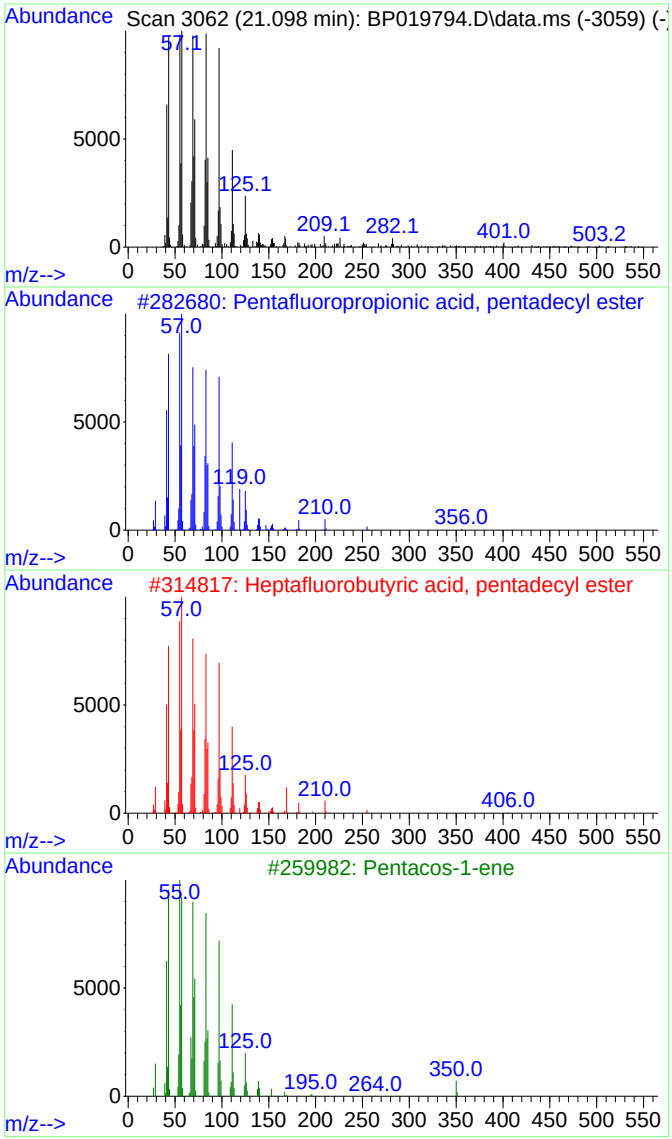
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

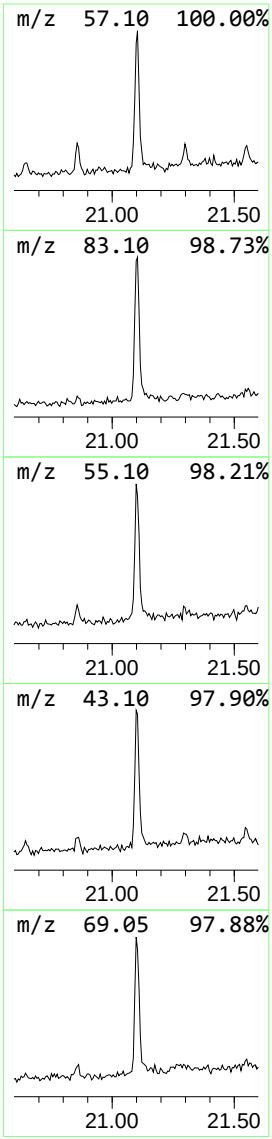
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Pentafluoropropionic acid, ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	3.91 ng	235264	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Nonacos-1-ene	406	C29H58	018835-35-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022024\
Data File : BP019794.D
Acq On : 20 Feb 2024 19:52
Operator : MA/JU
Sample : P1523-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240767-AMENDED-COMP-39N-N-3-02

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	117.9	ng	2173190	1	7.893	368704	20.0
2-Butenal, 2-me...	3.746	3.1	ng	57926	1	7.893	368704	20.0
2-Buten-1-ol, 2...	4.070	11.7	ng	215123	1	7.893	368704	20.0
2-Butenal, 3-me...	4.246	3.3	ng	60900	1	7.893	368704	20.0
Silane, trichlo...	4.305	3.6	ng	66745	1	7.893	368704	20.0
unknown4.452	4.452	4.0	ng	74524	1	7.893	368704	20.0
2-Pentanol, 4-m...	4.640	15.7	ng	289869	1	7.893	368704	20.0
unknown4.693	4.693	10.8	ng	198876	1	7.893	368704	20.0
2-Pentanone, 4-...	5.017	77.6	ng	1430650	1	7.893	368704	20.0
unknown6.099	6.099	2.7	ng	49938	1	7.893	368704	20.0
unknown6.722	6.722	3.1	ng	56510	1	7.893	368704	20.0
unknown7.593	7.593	3.9	ng	71128	1	7.893	368704	20.0
unknown8.863	8.863	3.2	ng	58658	1	7.893	368704	20.0
1,2-Benzenediol...	9.428	54.0	ng	1368260	2	10.699	506950	20.0
unknown13.299	13.299	4.5	ng	151308	3	14.528	670833	20.0
unknown14.451	14.451	2.8	ng	93584	3	14.528	670833	20.0
Hexathiane	15.140	2.9	ng	98725	3	14.528	670833	20.0
Lenthionine	16.263	7.5	ng	352333	4	17.287	938167	20.0
unknown17.063	17.063	4.0	ng	186998	4	17.287	938167	20.0
Pentafluoroprop...	21.098	3.9	ng	235264	5	21.380	1201920	20.0