LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20210589-AMENDED-COM-3

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.911	304	310	319	rVB	2278797	3252997	28.53%	4.196%
2	5.358	380	386	396	rBV	4549418	6418482	56.29%	8.280%
3	5.969	485	490	499	rVB	431753	626476	5.49%	0.808%
4	6.940	647	655	670	rVB	5074780	8041308	70.52%	10.373%
5	7.752	787	793	800	rBV	889609	1370004	12.01%	1.767%
6	8.910	982	990	999	rBV	3220242	5213028	45.71%	6.725%
7	9.263	1044	1050	1057	rBV	220703	382028	3.35%	0.493%
8	10.328	1224	1231	1241	rBV	823349	1273147	11.16%	1.642%
9	10.534	1258	1266	1272	rBV	1223199	1978286	17.35%	2.552%
10	10.881	1319	1325	1333	rBV	51781	118428	1.04%	0.153%
11	13.004	1677	1686	1700	rBV	6050172	9096006	79.77%	11.734%
12	13.128	1700	1707	1716	rVV	163381	285403	2.50%	0.368%
13	14.287	1897	1904	1914	rBV	360393	812908	7.13%	1.049%
14	14.381	1914	1920	1926	rVV	1676209	2505158	21.97%	3.232%
15	14.445	1926	1931	1939	rVB	113980	184255	1.62%	0.238%
16	14.998	2005	2025	2042	rBV2	63635	447479	3.92%	0.577%
17	15.428	2094	2098	2104	rVB2	84746	122268	1.07%	0.158%
18	15.875	2167	2174	2183	rBV	4337339	6036219	52.93%	7.787%
19	16.104	2207	2213	2221	rBV	896041	1338609	11.74%	1.727%
20	16.898	2341	2348	2354	rBV	1226969	1903927	16.70%	2.456%
21	17.134	2381	2388	2392	rBV	1895722	2787050	24.44%	3.595%
22	17.175	2392	2395	2401	rVB	607440	808706	7.09%	1.043%
23	17.263	2406	2410	2415	rVB	171273	235968	2.07%	0.304%
24	18.039	2538	2542	2549	rBV2	315673	436750	3.83%	0.563%
25	18.192	2563	2568	2572	rBV3	108925	188695	1.65%	0.243%
26	19.151	2726	2731	2736	rVB	732733	959346	8.41%	1.238%
27	19.275	2749	2752	2759	rBV3	86865	115524	1.01%	0.149%
28	19.475	2782	2786	2787	rBV2	138013	167031	1.46%	0.215%
29	19.498	2787	2790	2794	rVB	529615	672401	5.90%	0.867%
30	19.710	2820	2826	2831	rBV	9616350	11403427	100.00%	14.710%
31	19.986	2870	2873	2876	rVB2	106330	123663	1.08%	0.160%
32	20.086	2886	2890	2893	rBV	97306	120414	1.06%	0.155%
33	20.957	3033	3038	3044	rVB2	686618	920097	8.07%	1.187%
34	21.227	3078	3084	3088	rBV2	2429534	3438448	30.15%	4.436%
35	21.263	3088	3090	3098	rVB	303402	383093	3.36%	0.494%
36	21.392	3109	3112	3118	rVB3	194080	251962	2.21%	0.325%

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.845	3186	3189	3197	rVB2	157381	234232	2.05%	0.302%
38	23.557	3473	3480	3487	rBV2	1467634	2866320	25.14%	3.698%

Sum of corrected areas: 77519543

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
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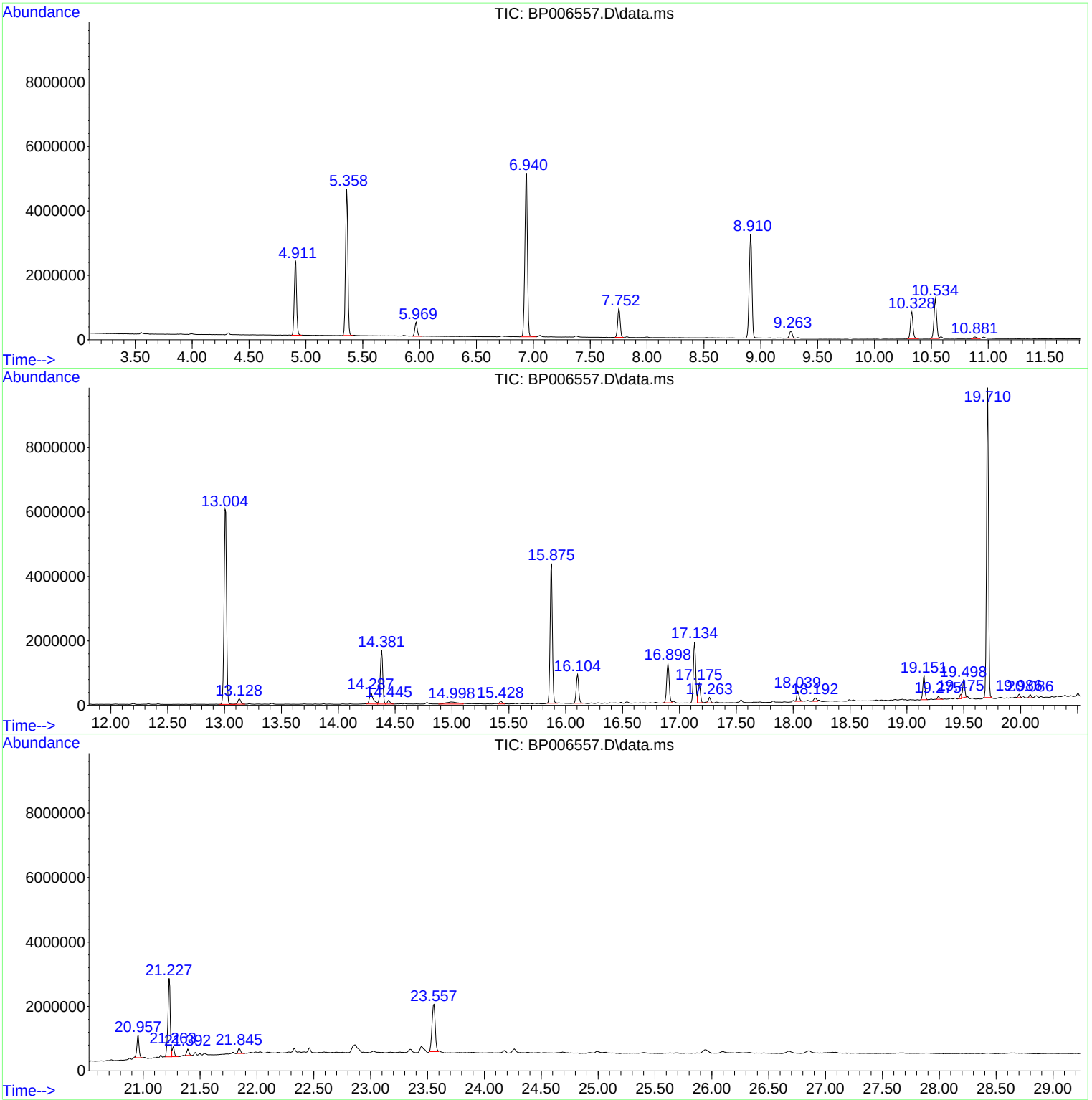
Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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\BP080621\
Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

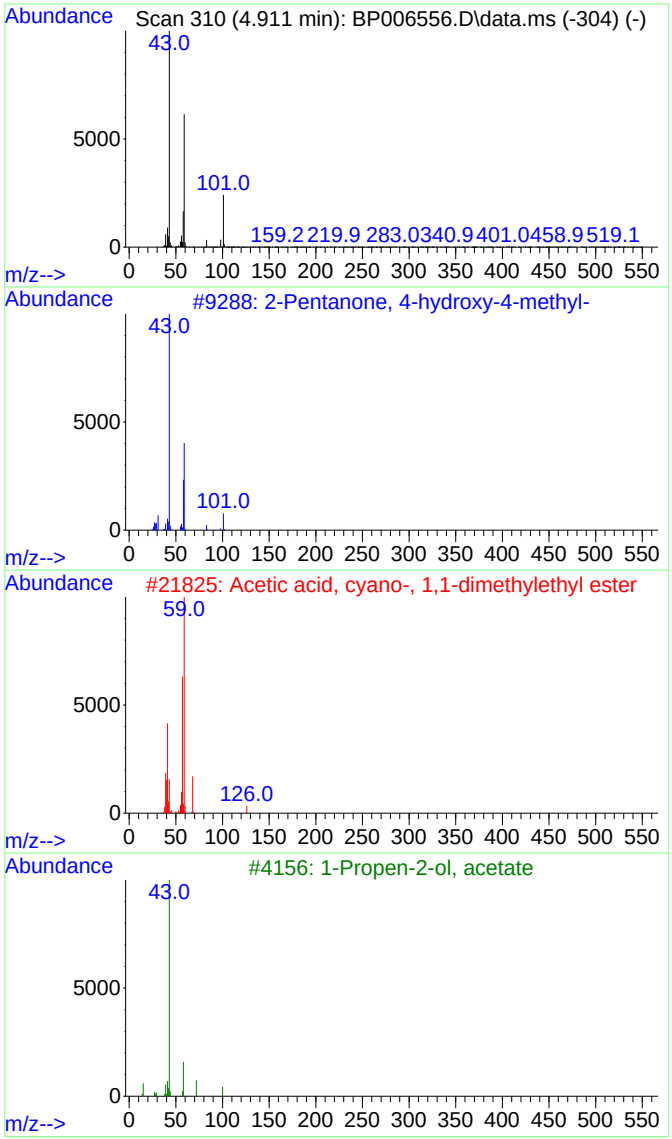
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

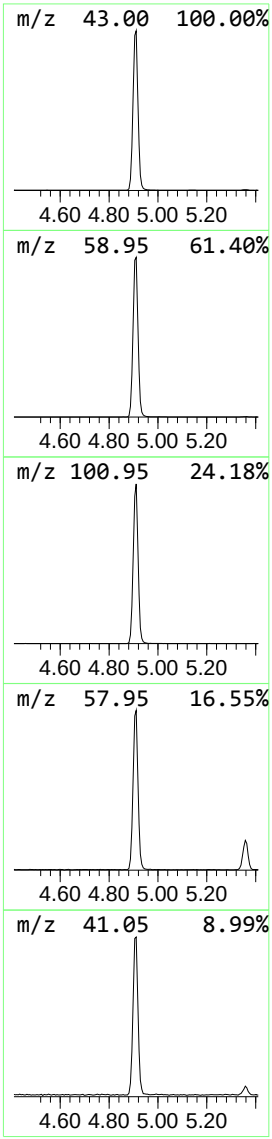
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.911	47.49 ng	3253000	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

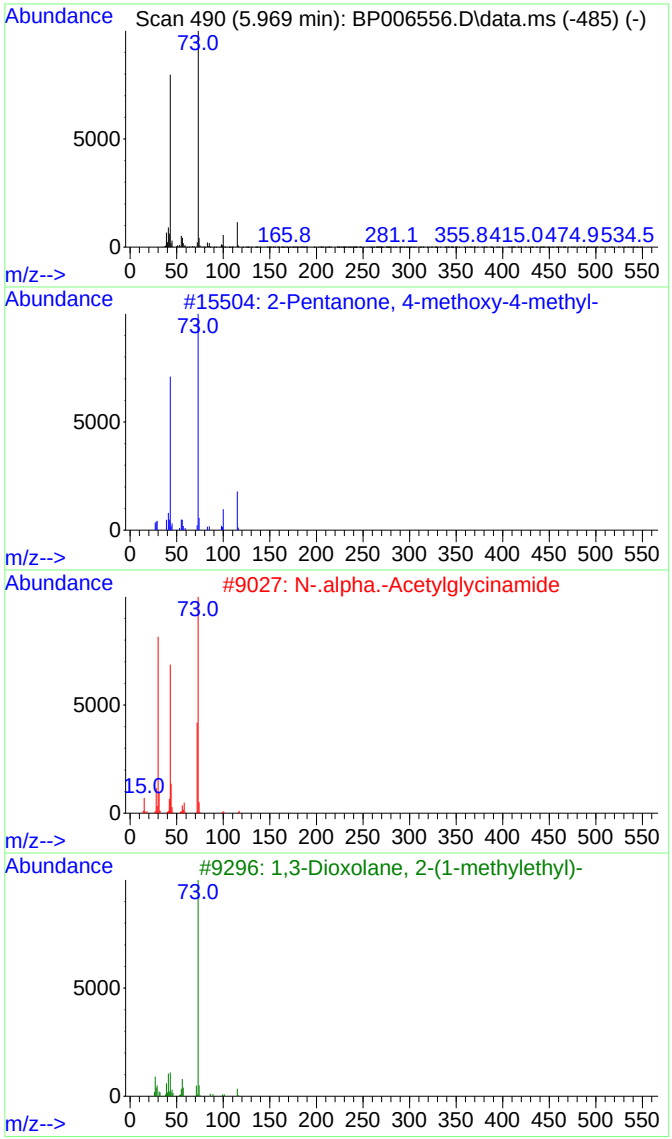
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

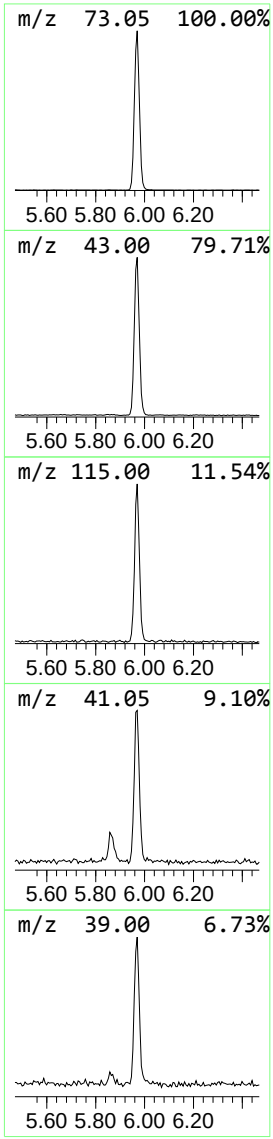
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	9.15 ng	626476	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

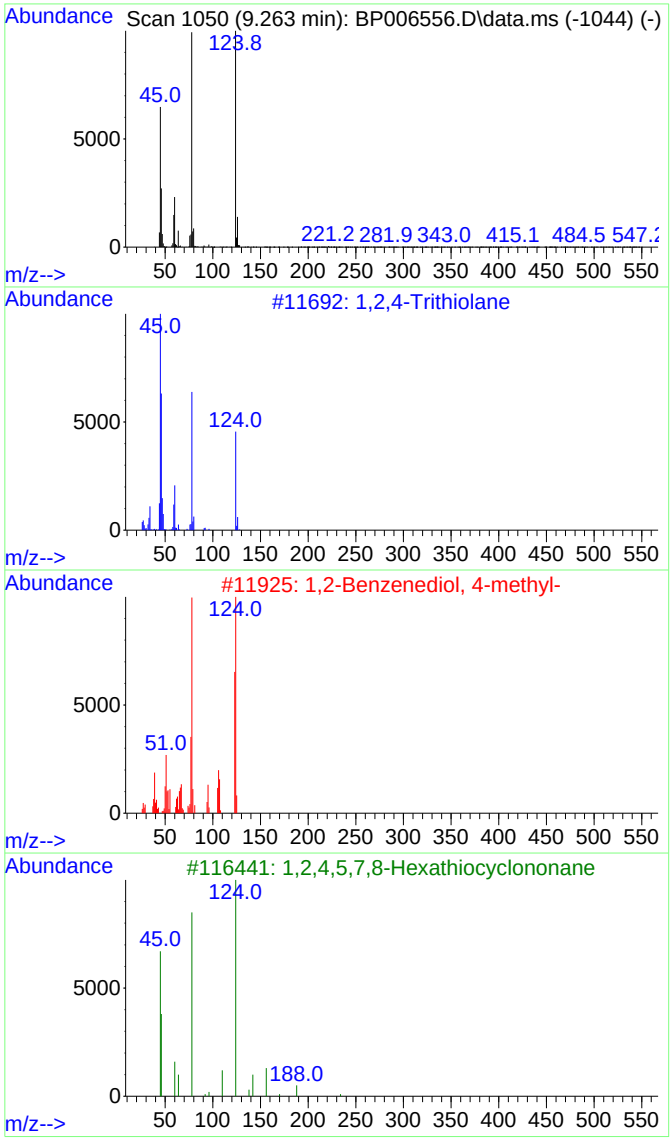
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

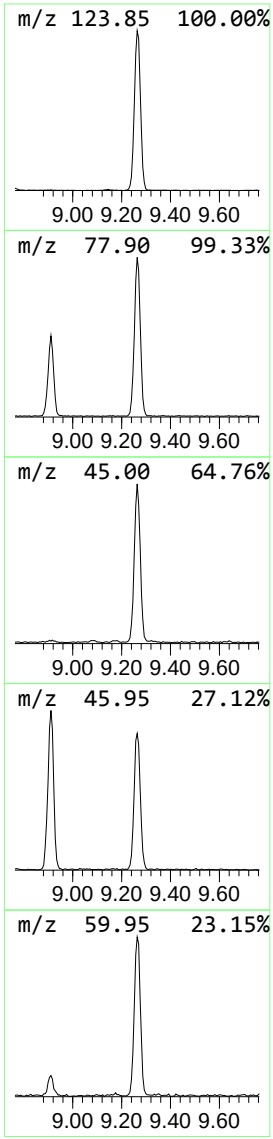
****

Peak Number 3 1,2,4-Trithiolane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	3.86 ng	382028	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	74
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
3	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
4	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	10
5	Benzene	78	C6H6	000071-43-2	9





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Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

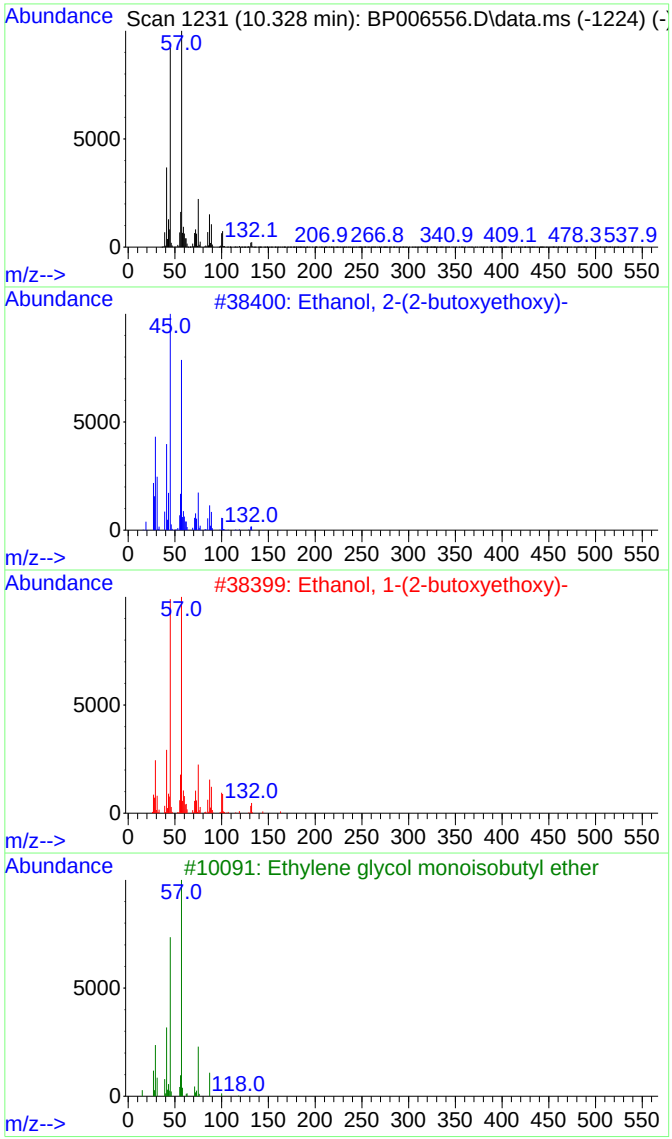
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

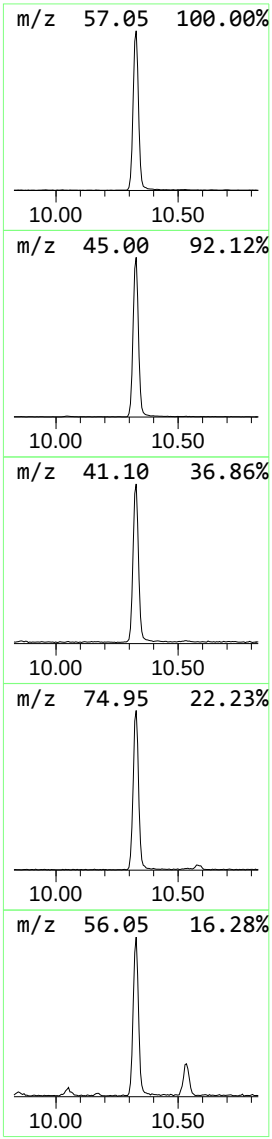
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	12.87 ng	1273150	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
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Acq On : 07 Aug 2021 01:37
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Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

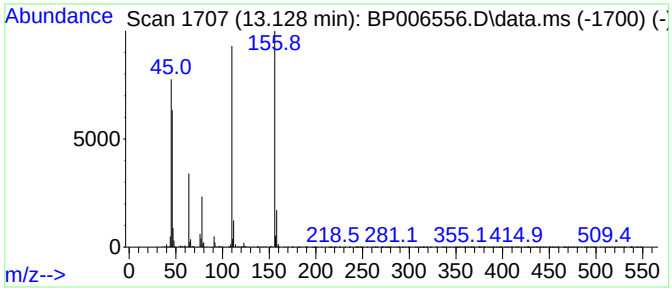
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

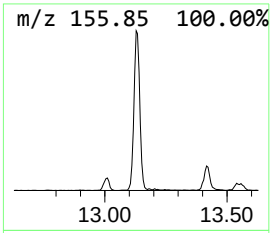
****

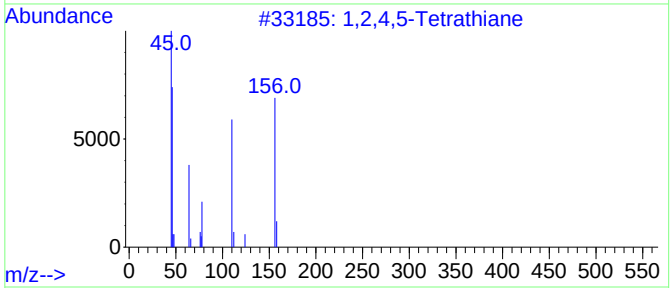
Peak Number 5 1,2,4,5-Tetrathiane Concentration Rank 11

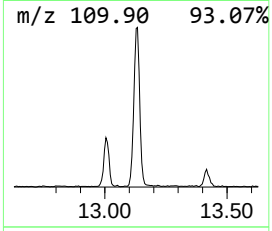
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	2.28 ng	285403	Acenaphthene-d10	14.381

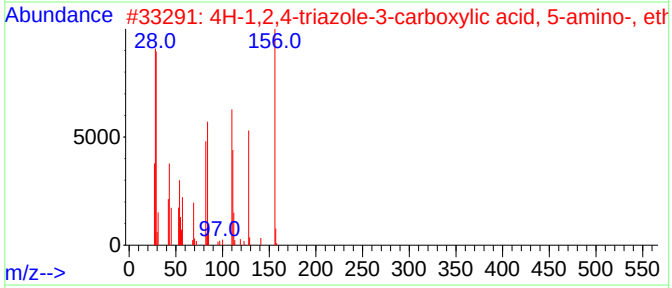
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane	156	C2H4S4	000291-22-5	59
2	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	25
3	Omethoate	213	C5H12NO4PS	001113-02-6	23
4	Methylene, bis(1,2,3,4-tetrahydr...	300	C9H8N4O4S2	1000276-89-7	10
5	2,3'-Dipyridyl	156	C10H8N2	000581-50-0	9

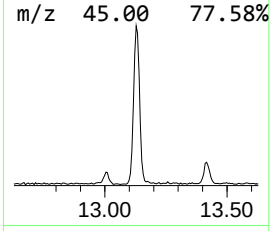


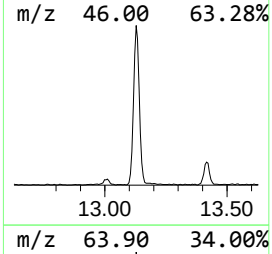


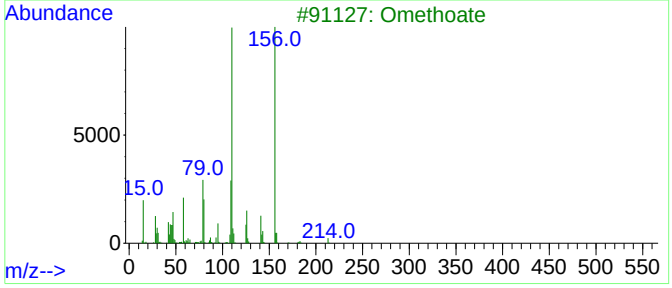


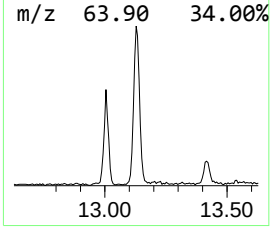












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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

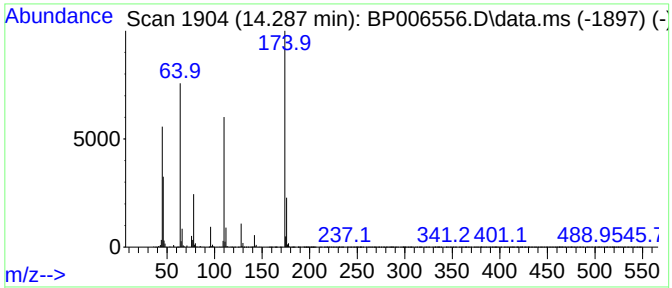
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

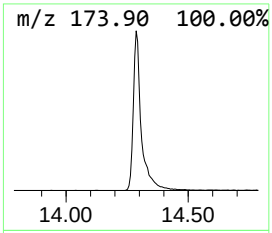
****

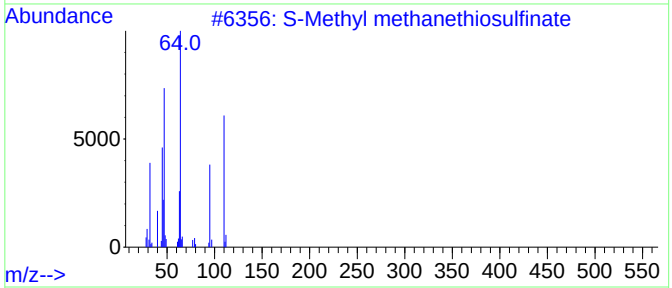
Peak Number 6 unknown14.287 Concentration Rank 6

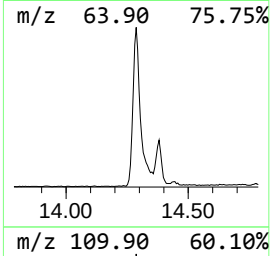
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.287	6.49 ng	812908	Acenaphthene-d10	14.381

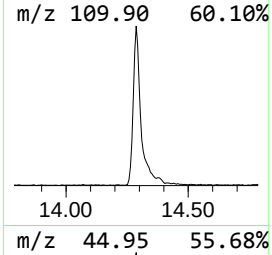
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	42
2	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	37
3	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	33
4	4-Pyridinesulfonamide 1-oxide	174	C5H6N2O3S	075903-65-0	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9

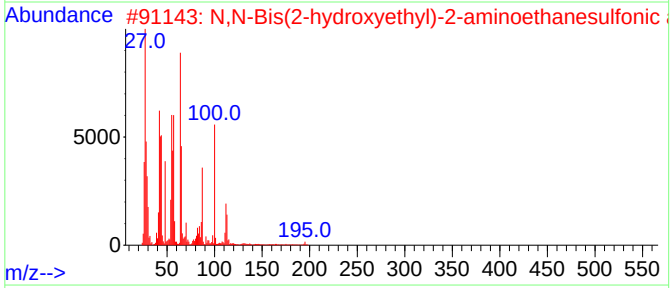


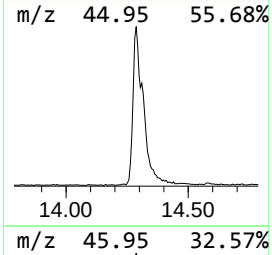


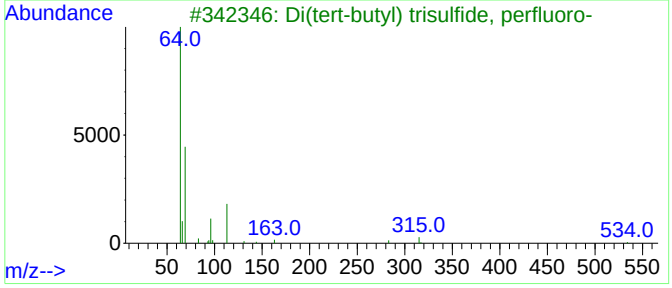


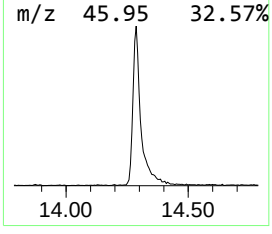












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Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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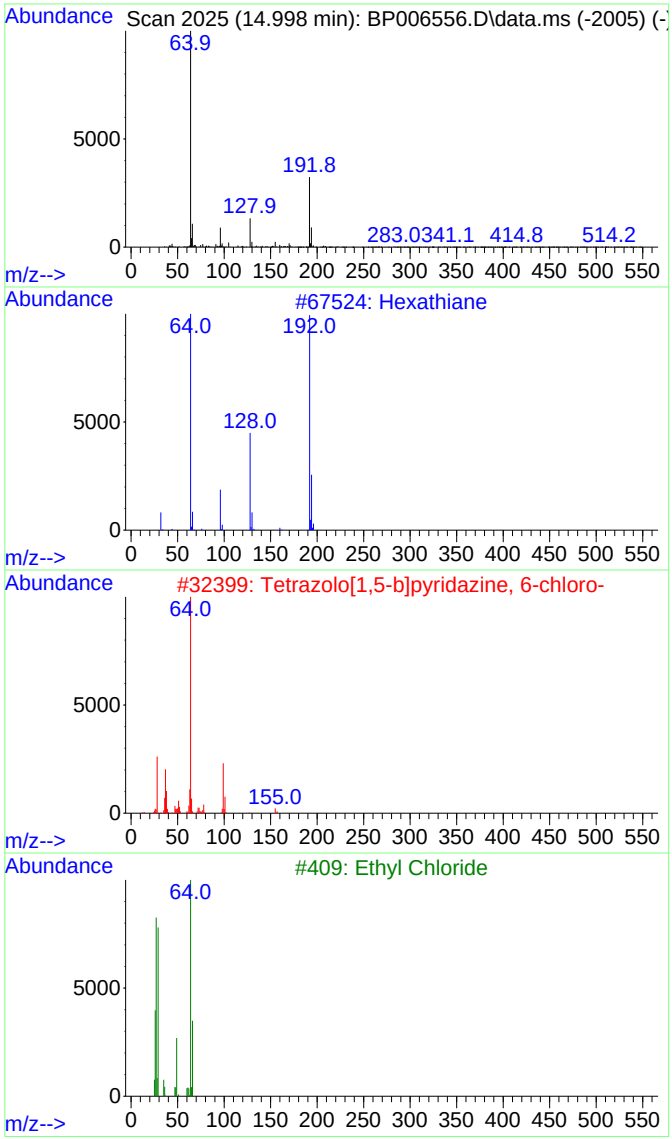
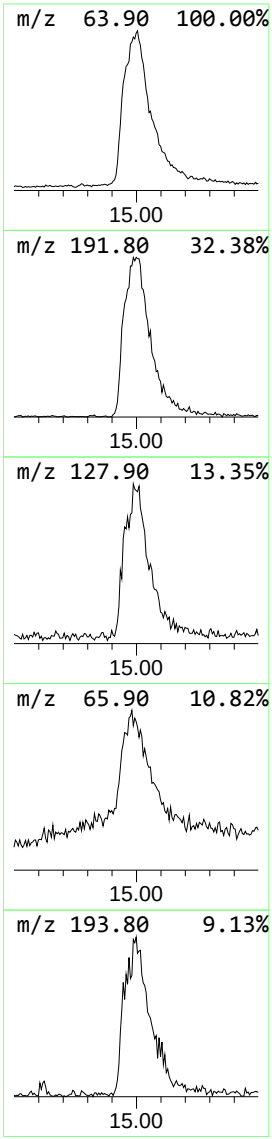
Peak Number 7 Hexathiane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	3.57 ng	447479	Acenaphthene-d10	14.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	7
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	5
4	Sulfur dioxide	64	O2S	007446-09-5	4
5	2,2,3,3-Tetrafluorocyclobutane-1...	153	C5H3F4N	1000487-04-1	4





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Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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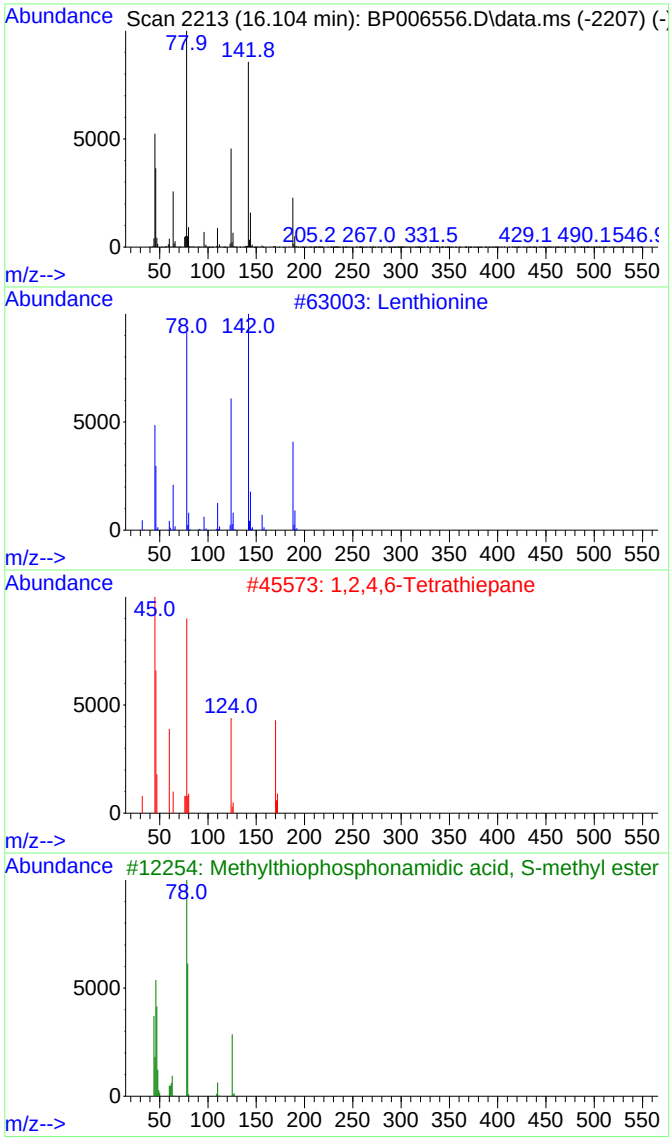
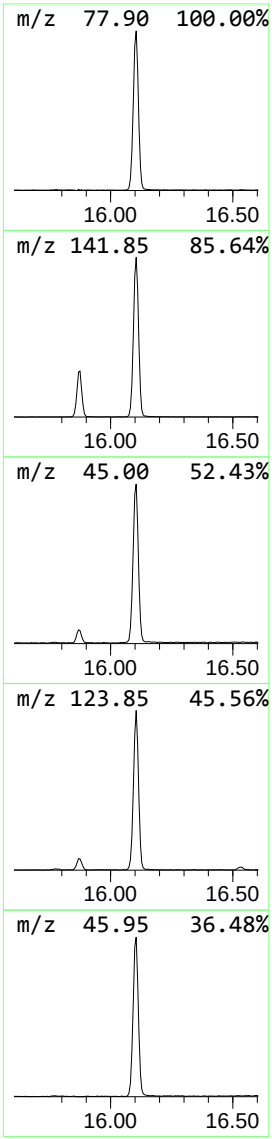
Peak Number 8 Lenthionine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	9.61 ng	1338610	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	95
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3	Methylthiophosphonamidic acid, S...	125	C2H8NOPS	1000306-03-2	9
4	Ethyl phenyl sulfoxide	154	C8H10OS	1000343-40-9	9
5	2,4-Hexadiyne	78	C6H6	002809-69-0	7





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Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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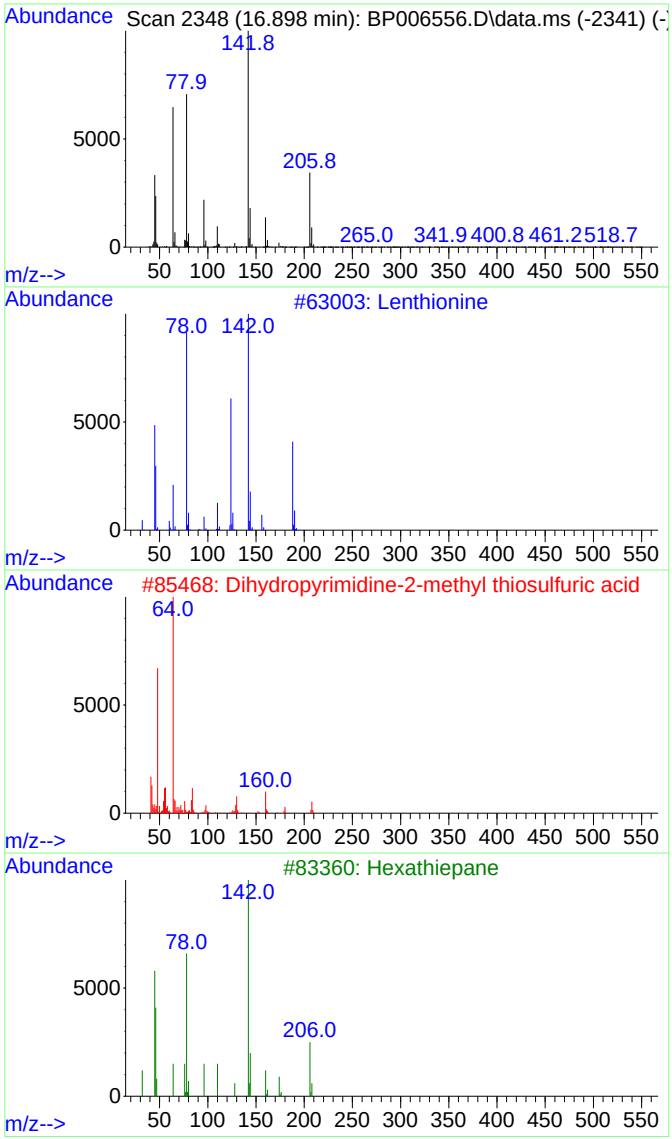
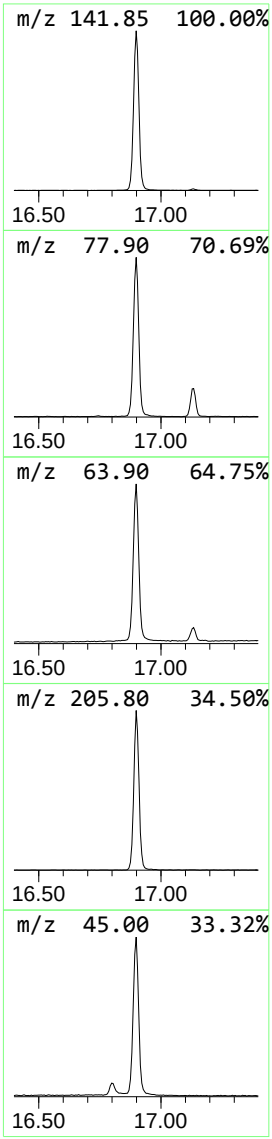
Peak Number 9 unknown16.898 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	13.66 ng	1903930	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	38
2	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	25
3	Hexathiepane	206	CH2S6	017233-71-5	25
4	1,3-Benzenedithiol	142	C6H6S2	000626-04-0	10
5	Benzenesulfinic-acid-	142	C6H6O2S	000618-41-7	9





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Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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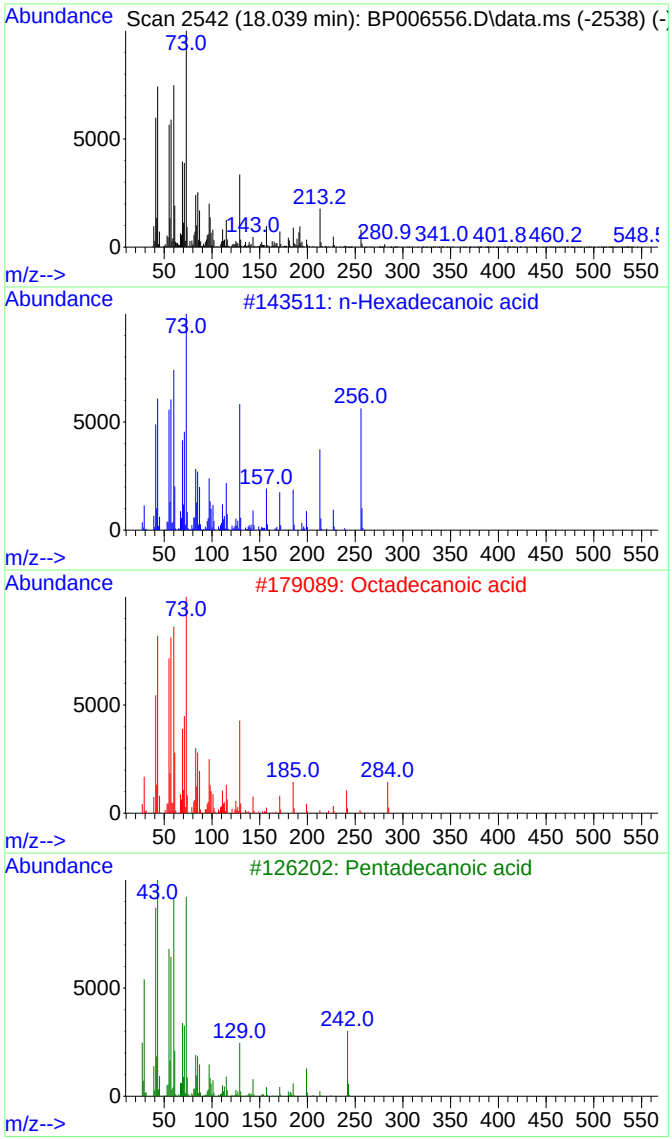
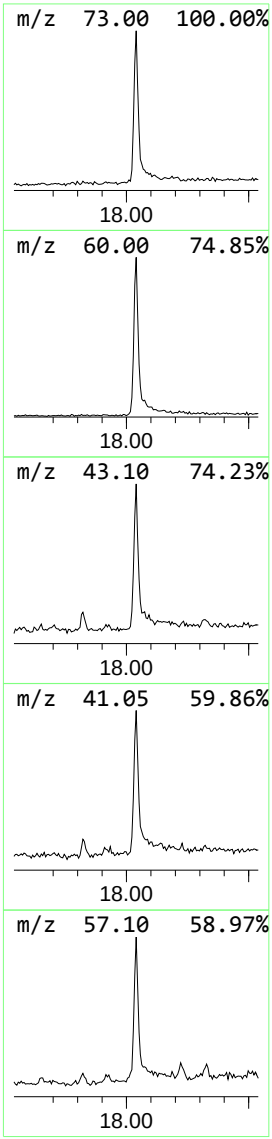
Peak Number 10 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	3.13 ng	436750	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Data File : BP006556.D
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Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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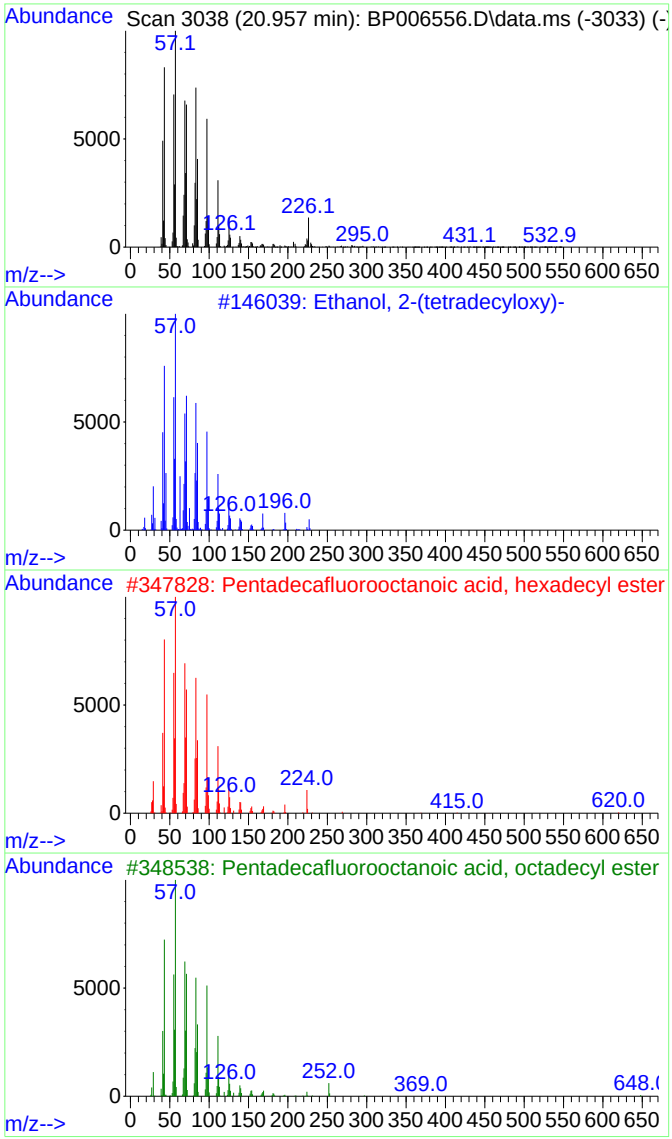
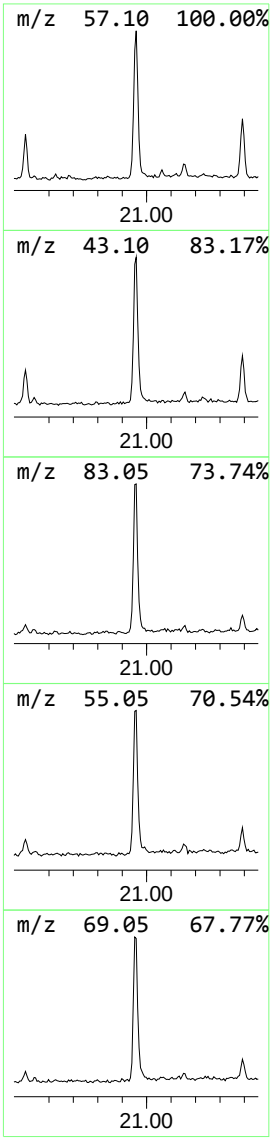
Peak Number 11 Ethanol, 2-(tetradecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	5.35 ng	920097	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	99
2	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Cyclohexadecane	224	C16H32	000295-65-8	89





Tentatively Identified Compound (LSC) summary

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Data File : BP006556.D
Acq On : 07 Aug 2021 01:37
Operator : CG/JU
Sample : M3279-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210589-AMENDED-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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
2-Pentanone, 4-...	4.911	47.5	ng	3253000	1	7.752	1370000	20.0
2-Pentanone, 4-...	5.969	9.2	ng	626476	1	7.752	1370000	20.0
1,2,4-Trithiolane	9.263	3.9	ng	382028	2	10.534	1978290	20.0
Ethanol, 2-(2-b...	10.328	12.9	ng	1273150	2	10.534	1978290	20.0
1,2,4,5-Tetrath...	13.128	2.3	ng	285403	3	14.381	2505160	20.0
unknown14.287	14.287	6.5	ng	812908	3	14.381	2505160	20.0
Hexathiane	14.998	3.6	ng	447479	3	14.381	2505160	20.0
Lenthionine	16.104	9.6	ng	1338610	4	17.134	2787050	20.0
unknown16.898	16.898	13.7	ng	1903930	4	17.134	2787050	20.0
n-Hexadecanoic ...	18.039	3.1	ng	436750	4	17.134	2787050	20.0
Ethanol, 2-(tet...	20.957	5.3	ng	920097	5	21.227	3438450	20.0