LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082525\
Data File : BP025577.D
Acq On : 25 Aug 2025 23:18
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
235

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-BP081425.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.037	12	17	22	rBV	1119104	1493165	21.46%	3.741%
2	4.943	335	341	350	rVB	494310	728652	10.47%	1.825%
3	5.414	412	421	428	rBV	2677058	4251090	61.11%	10.650%
4	6.978	675	687	699	rBV	2712347	4537601	65.22%	11.367%
5	7.784	816	824	829	rBV	954821	1518465	21.83%	3.804%
6	8.919	1009	1017	1028	rBV	1871363	3089262	44.41%	7.739%
7	10.484	1276	1283	1287	rBV3	114795	254902	3.66%	0.639%
8	10.549	1287	1294	1300	rVB	1166324	2024968	29.11%	5.073%
9	12.201	1568	1575	1583	rBV5	81764	221121	3.18%	0.554%
10	12.996	1704	1710	1717	rBV	4541336	6956960	100.00%	17.428%
11	13.160	1733	1738	1751	rBV4	250400	658766	9.47%	1.650%
12	13.813	1845	1849	1856	rVB3	232339	394827	5.68%	0.989%
13	13.925	1864	1868	1876	rBV2	345700	569693	8.19%	1.427%
14	14.043	1884	1888	1893	rBV	602092	887636	12.76%	2.224%
15	14.131	1896	1903	1909	rVV5	268820	720541	10.36%	1.805%
16	14.190	1910	1913	1915	rVV3	205577	286269	4.11%	0.717%
17	14.225	1916	1919	1925	rVB	504753	825718	11.87%	2.069%
18	14.390	1935	1947	1956	rVB	1726236	3682556	52.93%	9.225%
19	15.066	2059	2062	2068	rBV3	315857	465237	6.69%	1.165%
20	15.201	2081	2085	2088	rBV2	892690	1060887	15.25%	2.658%
21	15.907	2200	2205	2210	rBV	3170771	5289758	76.04%	13.252%

Sum of corrected areas: 39918074

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082525\
Data File : BP025577.D
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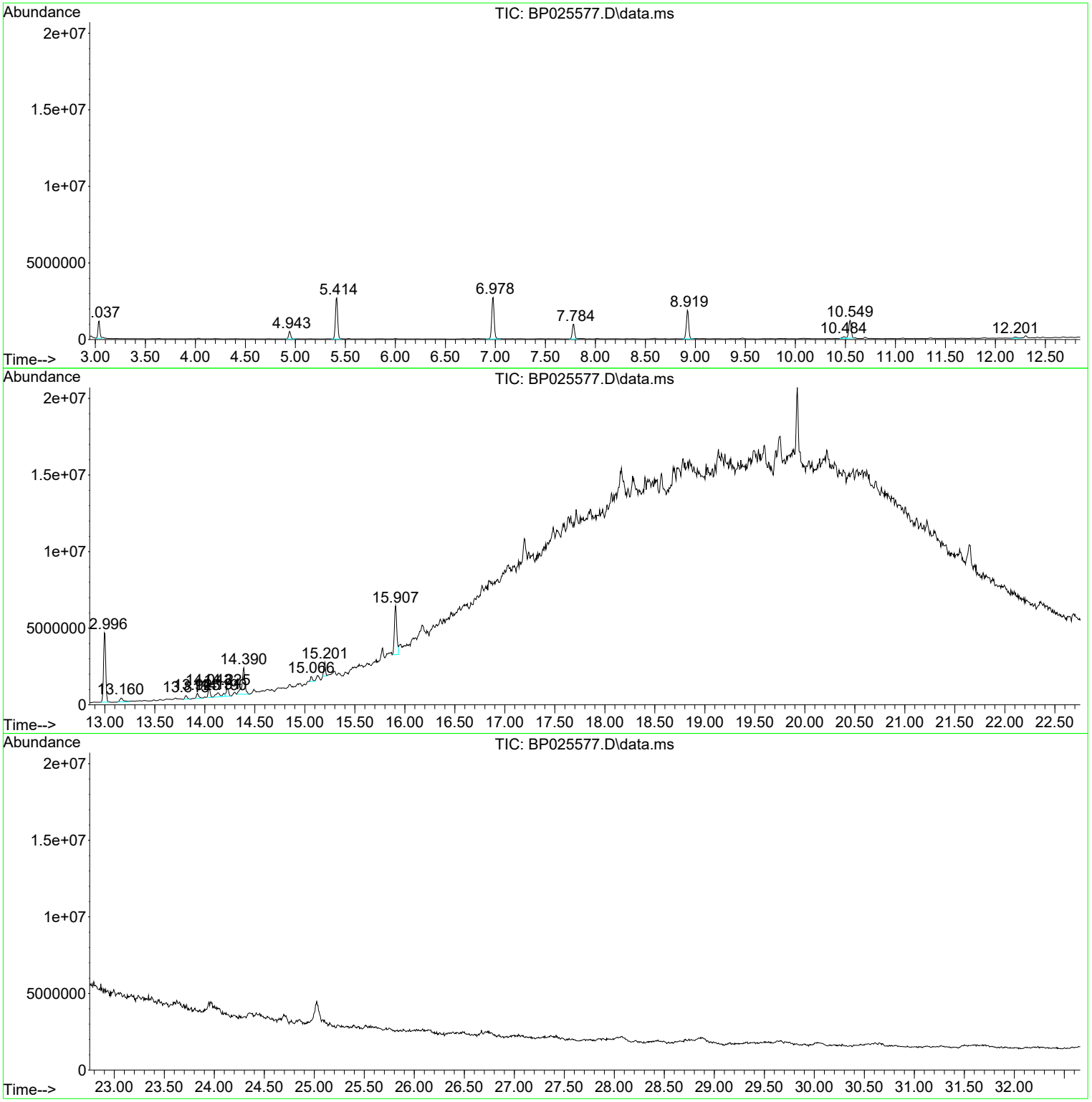
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
235

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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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Data File : BP025577.D
Acq On : 25 Aug 2025 23:18
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

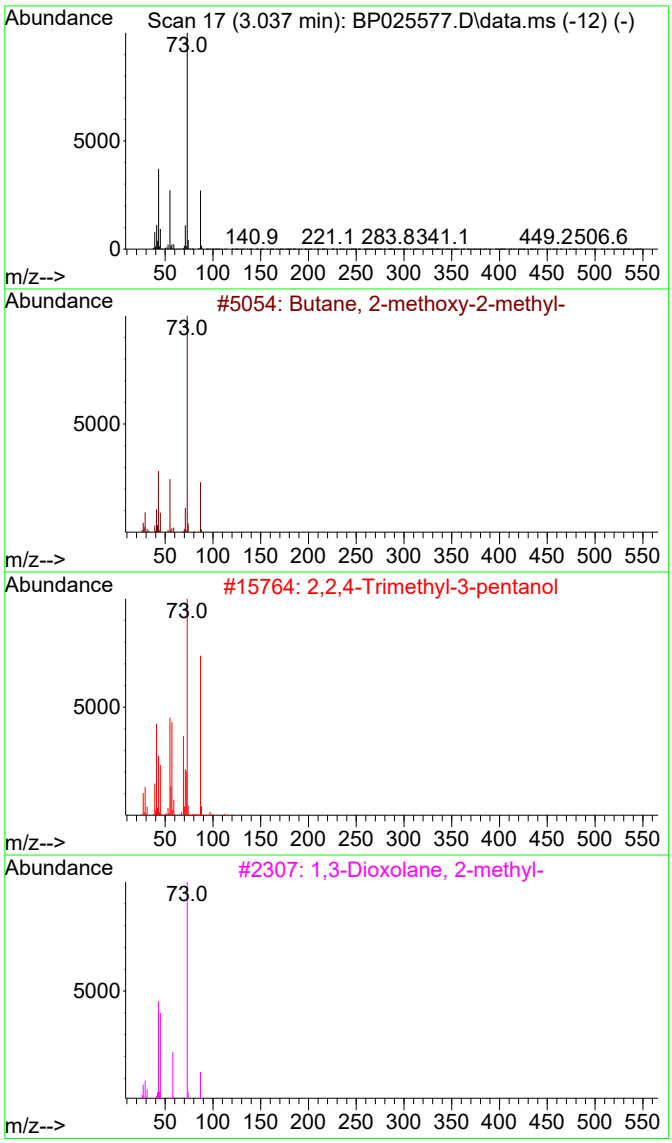
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

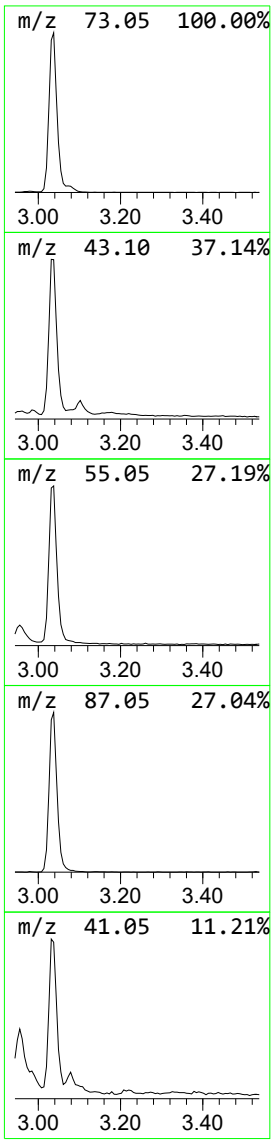
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.037	19.67 ng	1493170	1,4-Dichlorobenzene-d4	7.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : CG/JU
Sample : Q2947-03
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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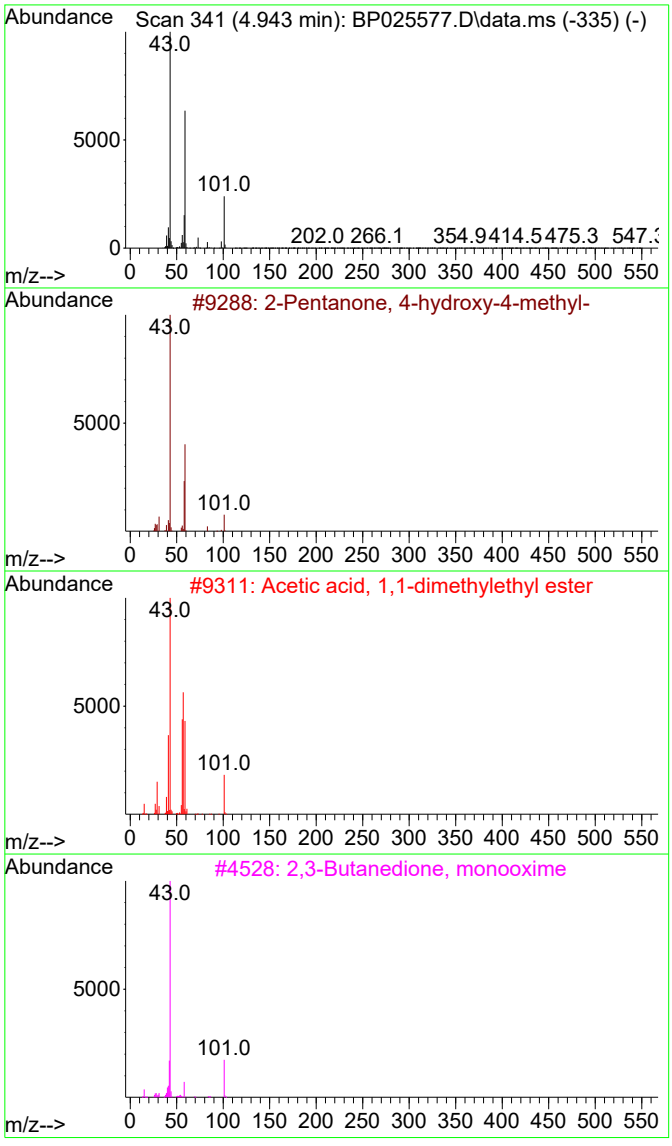
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

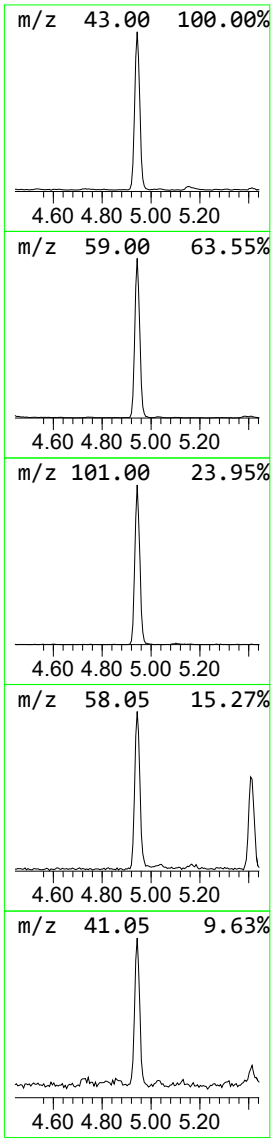
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.943	9.60 ng	728652	1,4-Dichlorobenzene-d4	7.784

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32





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Data File : BP025577.D
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Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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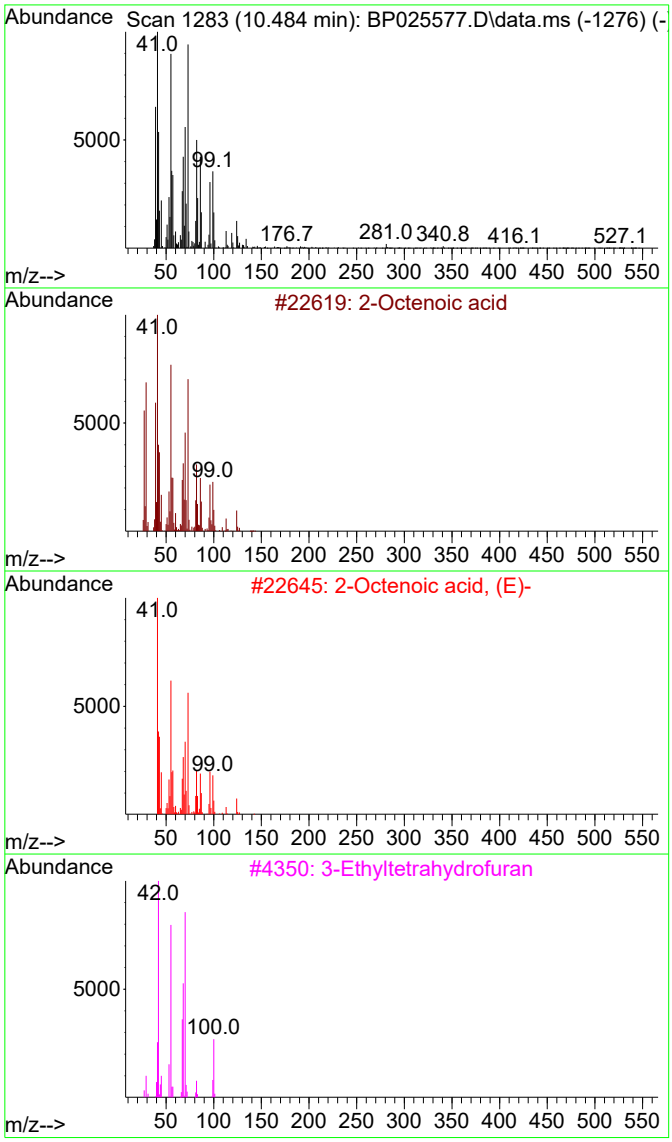
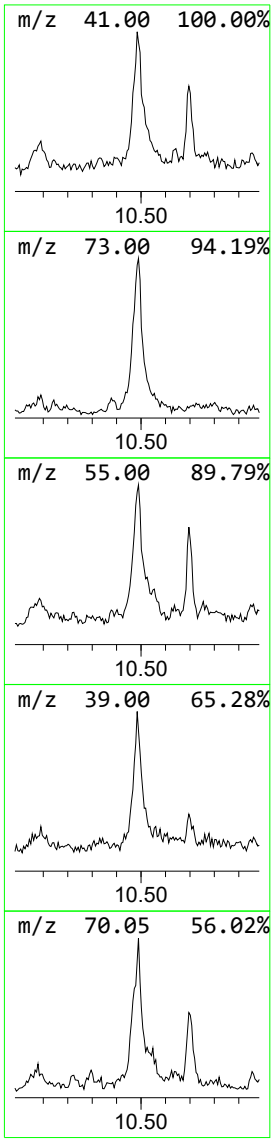
****

Peak Number 3 2-Octenoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.484	2.52 ng	254902	Naphthalene-d8	10.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenoic acid	142	C8H14O2	001470-50-4	94
2	2-Octenoic acid, (E)-	142	C8H14O2	001871-67-6	90
3	3-Ethyltetrahydrofuran	100	C6H12O	093716-28-0	43
4	Hexanoic acid, undec-10-enyl ester	268	C17H32O2	1010279-26-4	38
5	E-1,9-Hexadecadiene	222	C16H30	1000245-71-4	35





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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

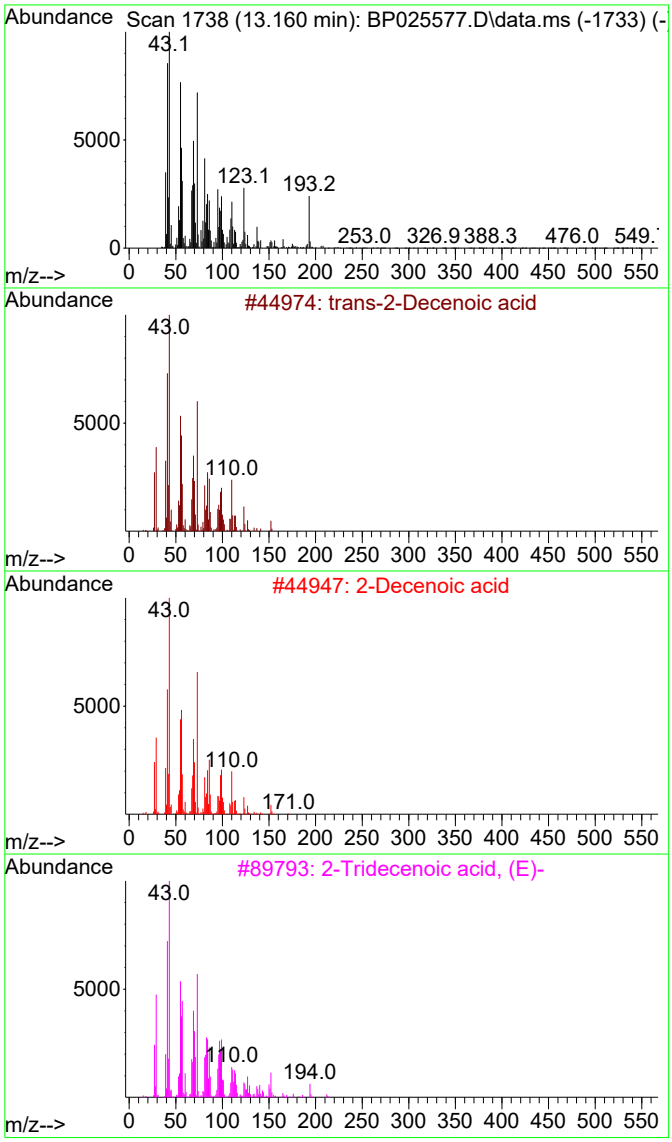
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

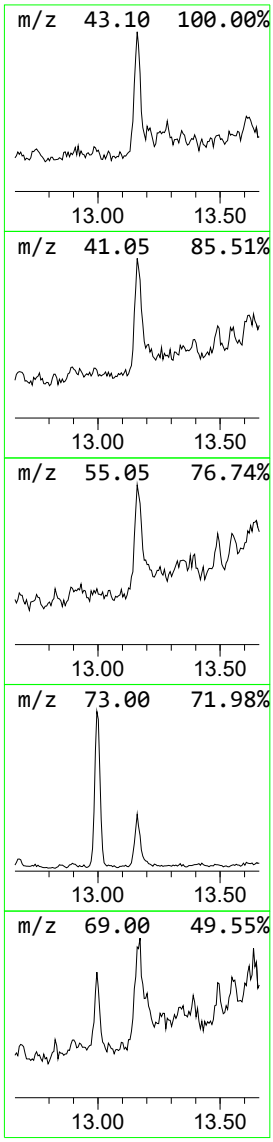
****

Peak Number 5 trans-2-Decenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.160	3.58 ng	658766	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Decenoic acid	170	C10H18O2	000334-49-6	58
2	2-Decenoic acid	170	C10H18O2	003913-85-7	46
3	2-Tridecenoic acid, (E)-	212	C13H24O2	032466-55-0	27
4	E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	25
5	2-Heptenoic acid	128	C7H12O2	018999-28-5	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082525\
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
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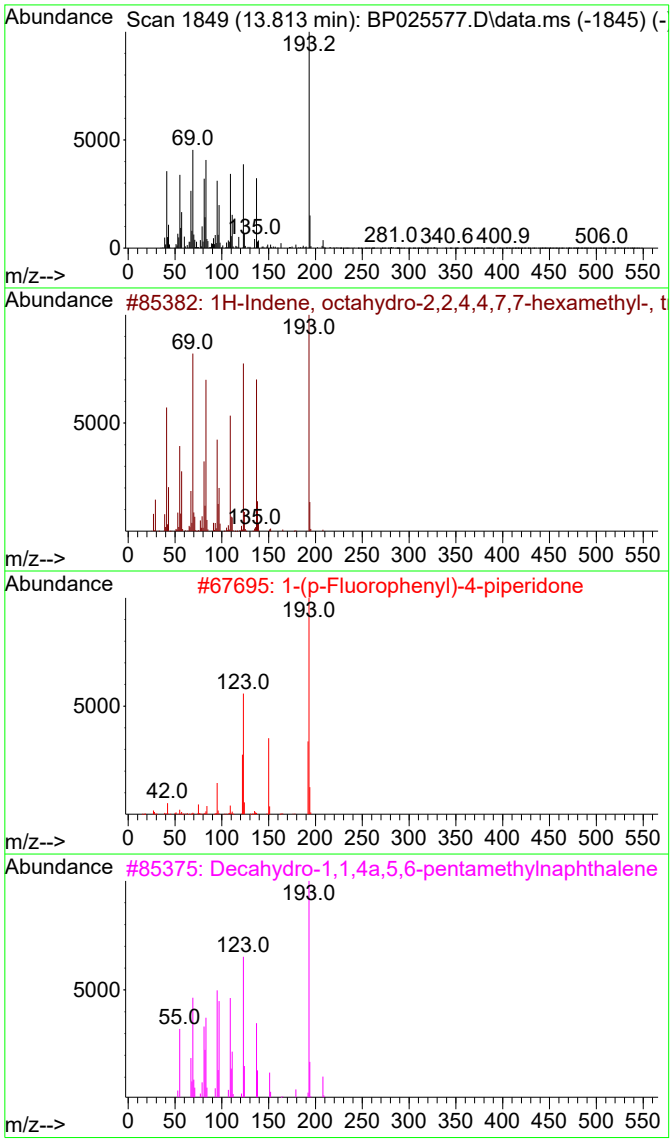
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

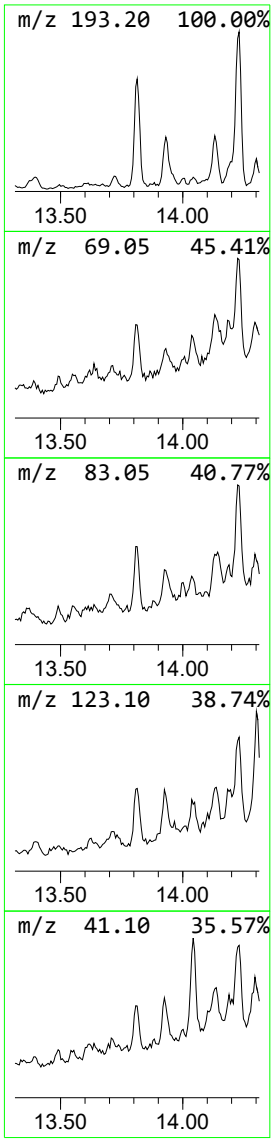
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, octahydro-2,2,4,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.813	2.14 ng	394827	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	37
5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	30





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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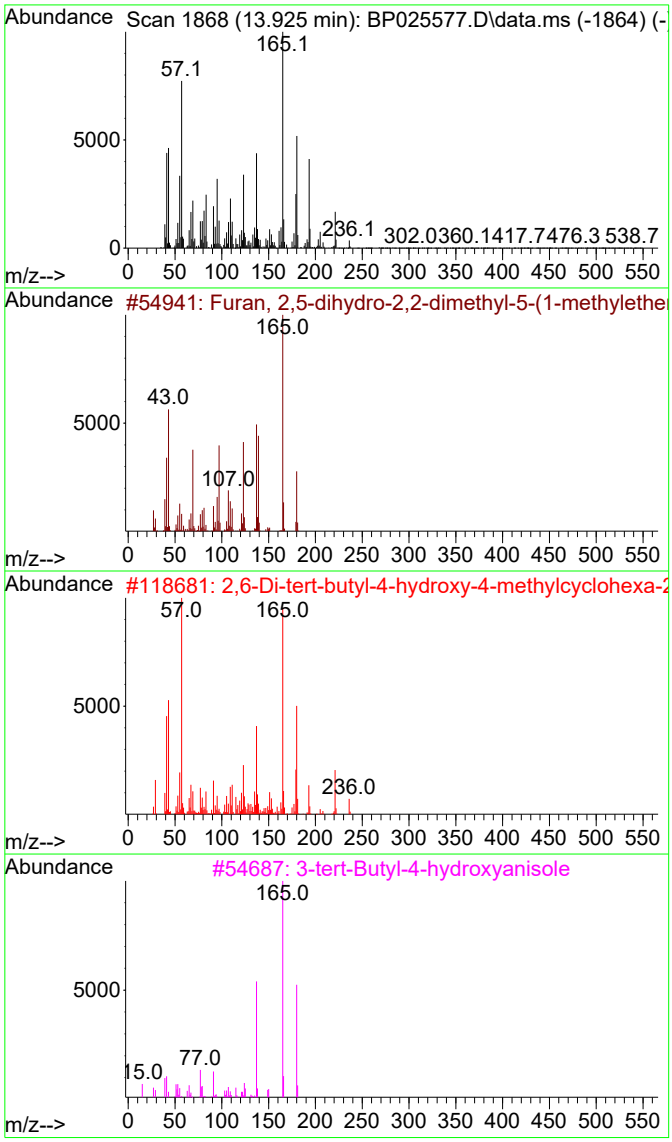
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

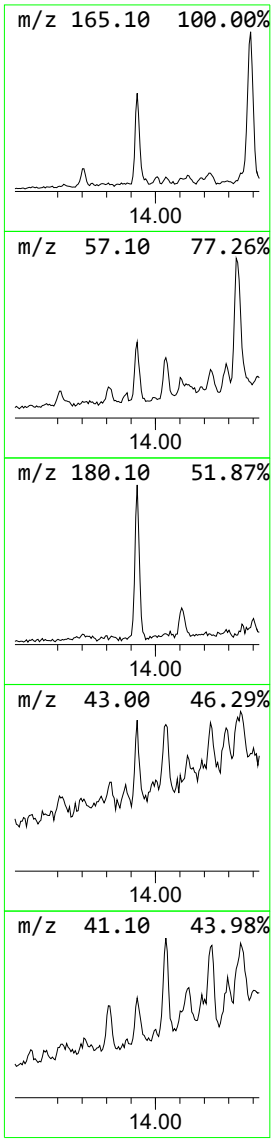
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Furan, 2,5-dihydro-2,2-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.925	3.09 ng	569693	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-2,2-dimethyl-...	180	C12H20O	077822-53-8	58
2	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	58
3	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	55
4	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	55
5	p-Cresol, TMS derivative	180	C10H16OSi	017902-32-8	38





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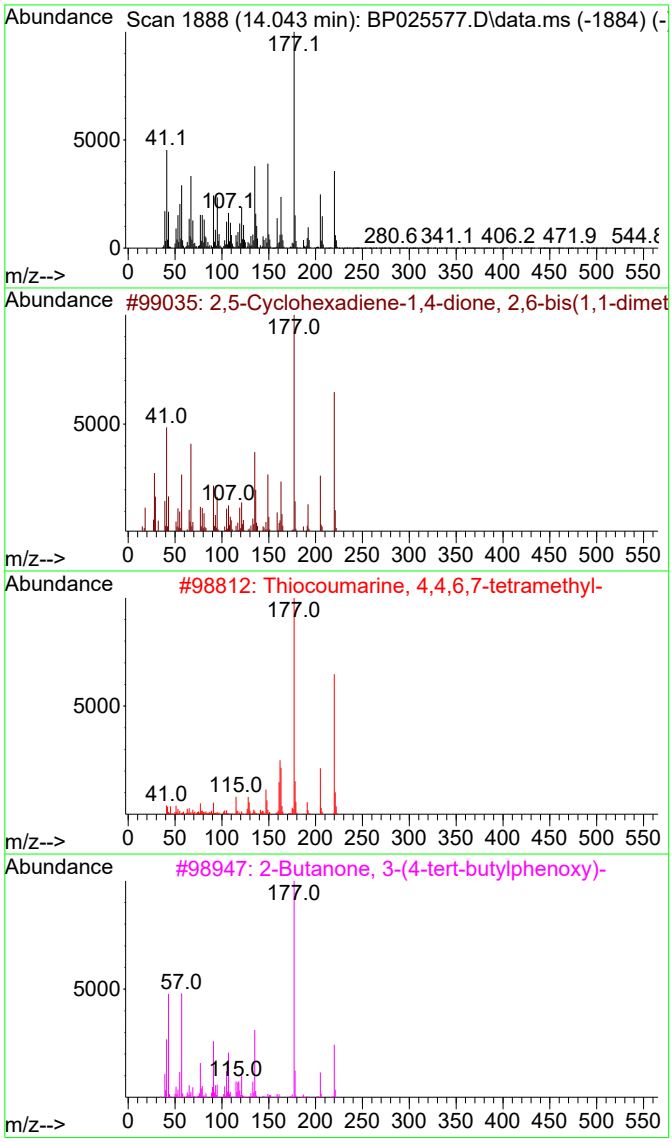
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

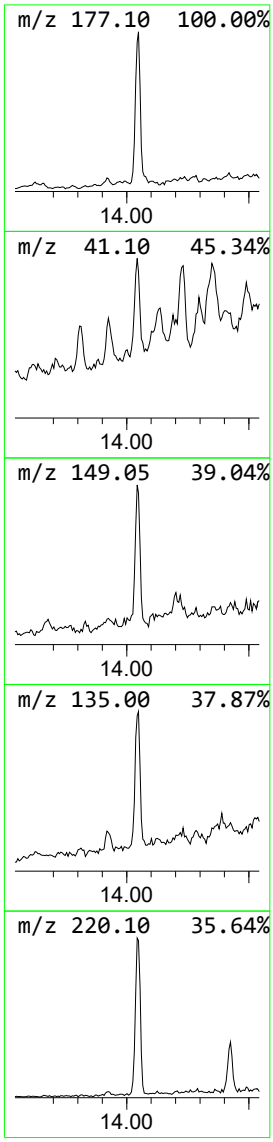
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.043	4.82 ng	887636	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	60
3	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	55
4	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	50
5	Benzofuran-2-one, 4-amino-2,3-di...	177	C10H11NO2	1000129-51-7	43





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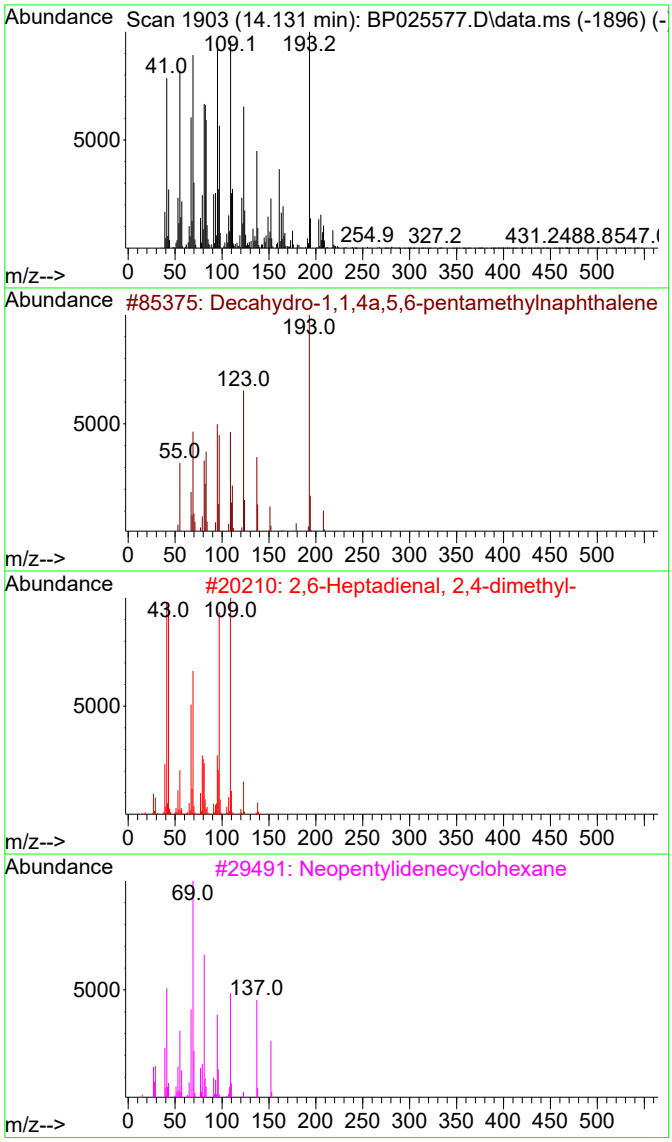
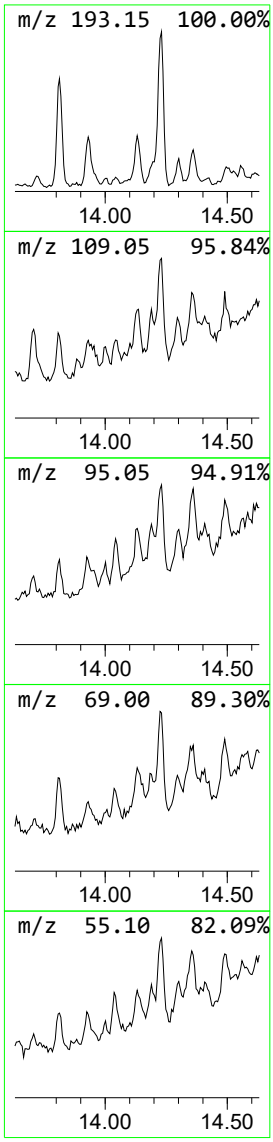
****

Peak Number 9 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.131	3.91 ng	720541	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	70
2	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
3	Neopentylidenecyclohexane	152	C11H20	039546-80-0	25
4	1-Anthracenamine	193	C14H11N	000610-49-1	20
5	3-Hexadecyne	222	C16H30	061886-62-2	20





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TIC Library : C:\Database\NIST20.L
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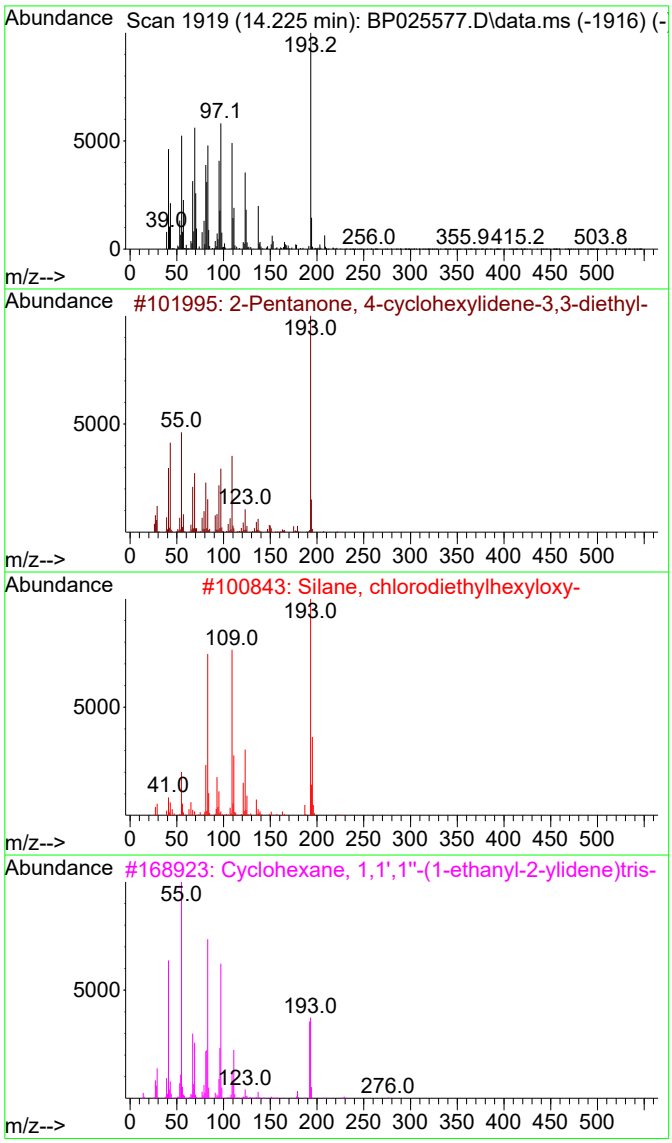
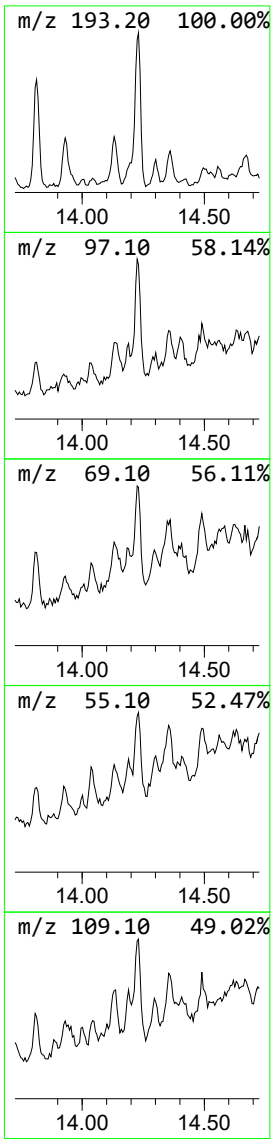
****

Peak Number 10 unknown14.225 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	4.48 ng	825718	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	40
3	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	38
4	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	22
5	2-Phenylindolizine	193	C14H11N	025379-20-8	14





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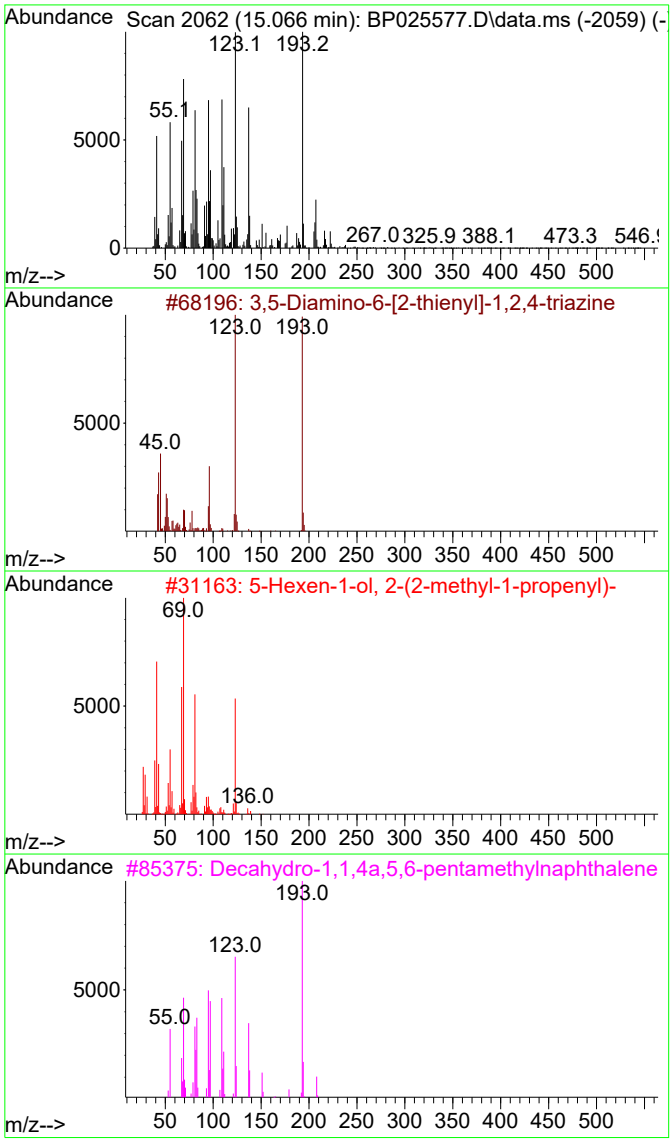
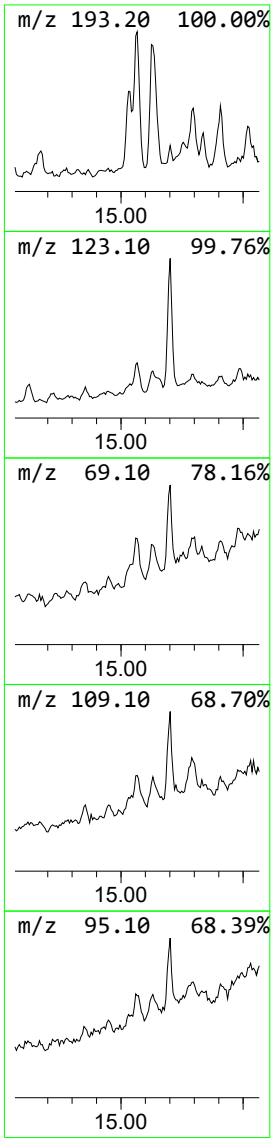
****

Peak Number 11 unknown15.066 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.066	2.53 ng	465237	Acenaphthene-d10	14.390

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S	058848-66-1	30
2	5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	27
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	22
4	2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	20
5	Benzeneacetic acid, 4-fluoro-.al...	168	C8H5FO3	002251-76-5	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082525\
Data File : BP025577.D
Acq On : 25 Aug 2025 23:18
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
235

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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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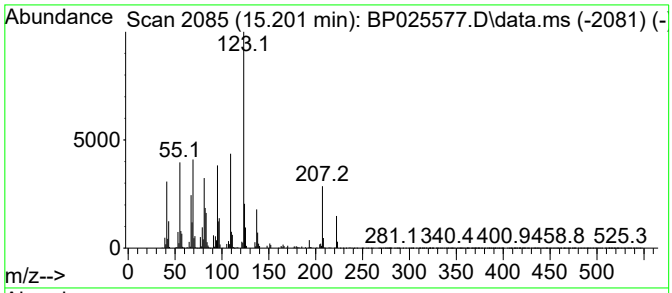
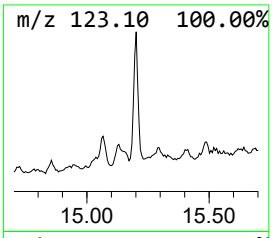
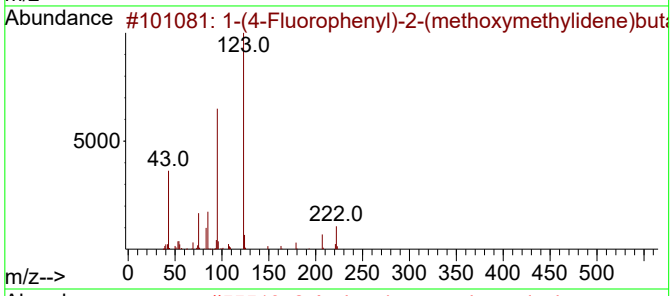
Peak Number 12 unknown15.201 Concentration Rank 3

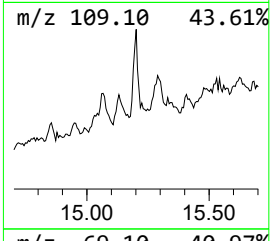
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.201	5.76 ng	1060890	Acenaphthene-d10	14.390

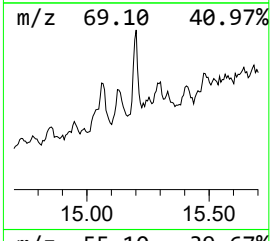
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	47
2	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	43
3	Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	43
4	4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	43
5	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	43

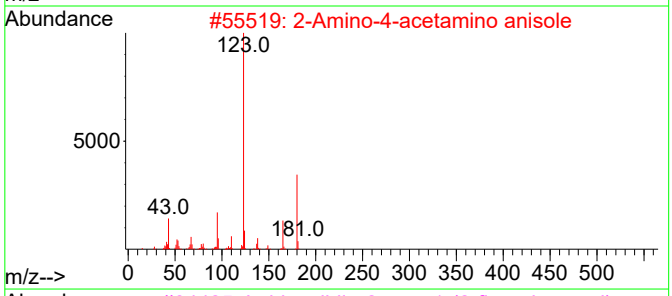


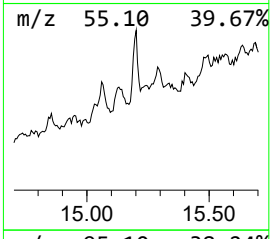


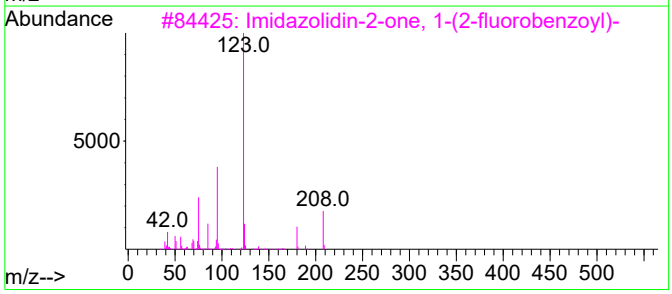


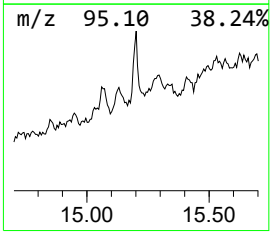












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082525\
Data File : BP025577.D
Acq On : 25 Aug 2025 23:18
Operator : CG/JU
Sample : Q2947-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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
Butane, 2-metho...	3.037	19.7	ng	1493170	1	7.784	1518470	20.0
2-Pentanone, 4-...	4.943	9.6	ng	728652	1	7.784	1518470	20.0
2-Octenoic acid	10.484	2.5	ng	254902	2	10.549	2024970	20.0
trans-2-Decenoi...	13.160	3.6	ng	658766	3	14.390	3682560	20.0
1H-Indene, octa...	13.813	2.1	ng	394827	3	14.390	3682560	20.0
Furan, 2,5-dihy...	13.925	3.1	ng	569693	3	14.390	3682560	20.0
2,5-Cyclohexadi...	14.043	4.8	ng	887636	3	14.390	3682560	20.0
Decahydro-1,1,4...	14.131	3.9	ng	720541	3	14.390	3682560	20.0
unknown14.225	14.225	4.5	ng	825718	3	14.390	3682560	20.0
unknown15.066	15.066	2.5	ng	465237	3	14.390	3682560	20.0
unknown15.201	15.201	5.8	ng	1060890	3	14.390	3682560	20.0