LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

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-BP082622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.322	53	57	67	rBV	188568	270976	1.73%	0.492%
2	4.699	286	291	299	rBV	186033	252495	1.62%	0.458%
3	5.146	358	367	377	rBV	1263982	1874713	12.00%	3.404%
4	6.734	631	637	647	rBV	806843	1291012	8.26%	2.344%
5	7.540	766	774	782	rBV	395472	623485	3.99%	1.132%
6	7.846	814	826	832	rBV2	220490	525846	3.37%	0.955%
7	8.557	929	947	950	rBV4	174478	492302	3.15%	0.894%
8	8.663	957	965	968	rBV	361890	778640	4.98%	1.414%
9	8.710	968	973	981	rVB	1696859	2863143	18.32%	5.198%
10	9.351	1078	1082	1095	rVB	131214	232051	1.49%	0.421%
11	10.328	1242	1248	1254	rBV	574538	924654	5.92%	1.679%
12	12.286	1577	1581	1589	rVV	90718	220767	1.41%	0.401%
13	12.363	1589	1594	1604	rVB3	112741	245259	1.57%	0.445%
14	12.828	1664	1673	1680	rBV	3966745	5751096	36.81%	10.441%
15	13.239	1737	1743	1754	rBV	108608	187093	1.20%	0.340%
16	14.216	1903	1909	1916	rBV	885603	1285720	8.23%	2.334%
17	15.722	2159	2165	2177	rBV	4098908	5605391	35.87%	10.177%
18	16.986	2374	2380	2389	rBV	1143975	1591963	10.19%	2.890%
19	17.910	2533	2537	2546	rBV	164627	265286	1.70%	0.482%
20	19.586	2817	2822	2833	rVB	8322765	9859781	63.10%	17.900%
21	20.845	3032	3036	3043	rBV	363017	495423	3.17%	0.899%
22	21.115	3077	3082	3086	rBV	1550022	1847215	11.82%	3.354%
23	21.257	3100	3106	3131	rBV	11677983	15625366	100.00%	28.368%
24	23.398	3464	3470	3481	rVB2	1059299	1971814	12.62%	3.580%

Sum of corrected areas: 55081491

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
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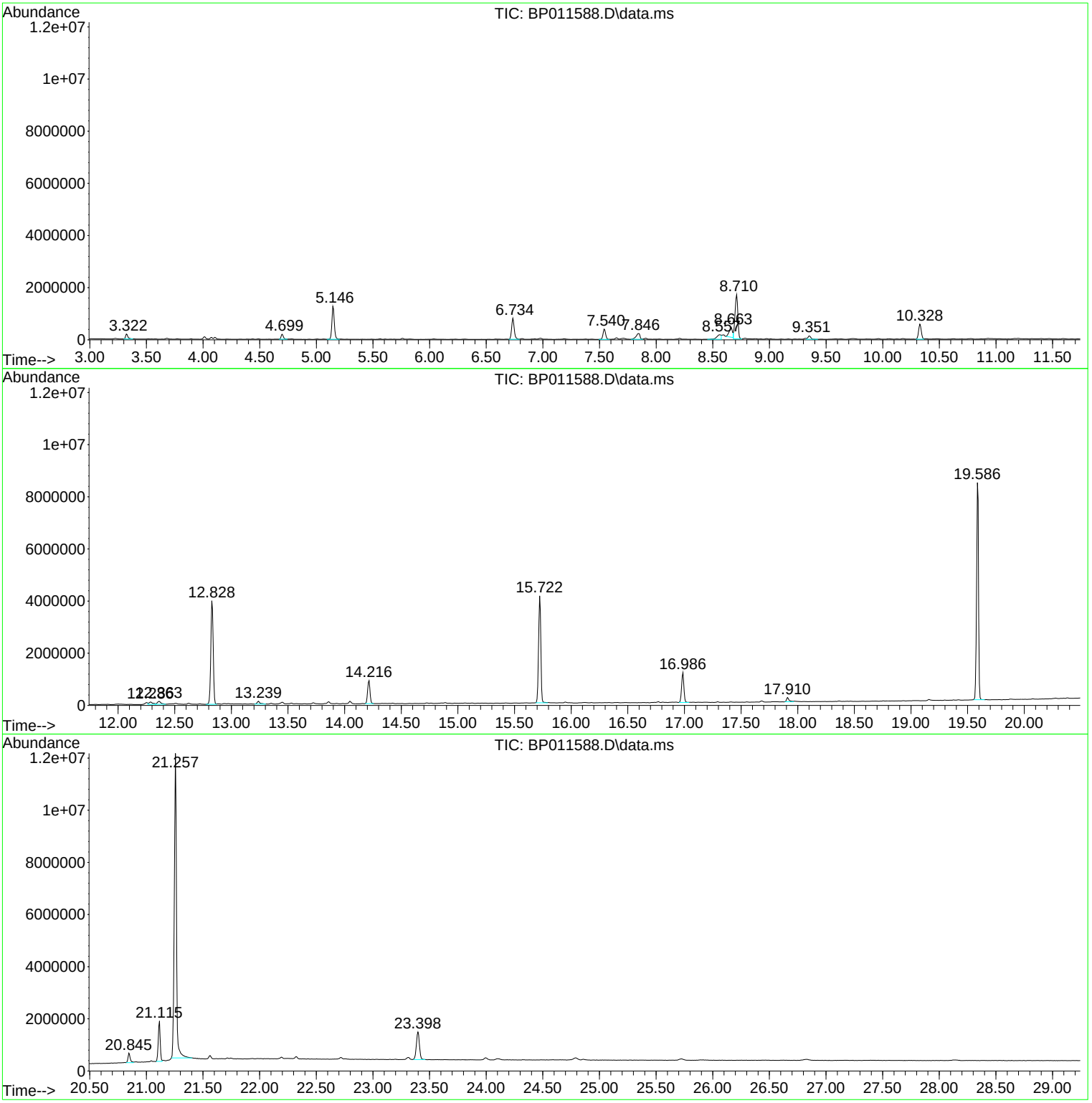
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.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\BP082622\
Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

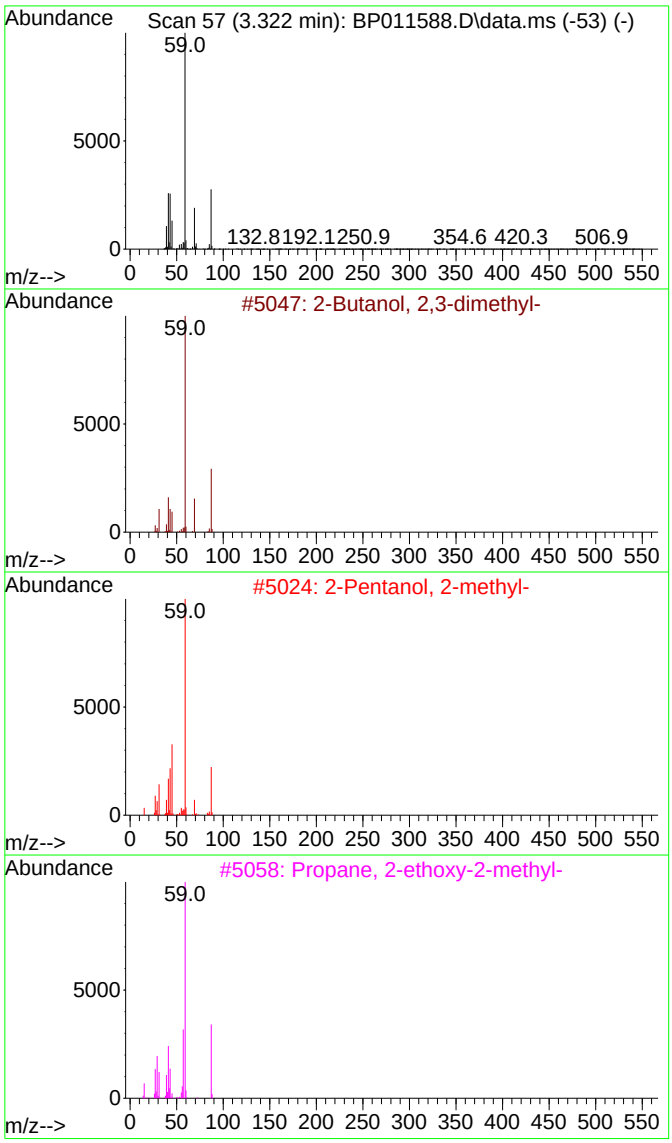
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

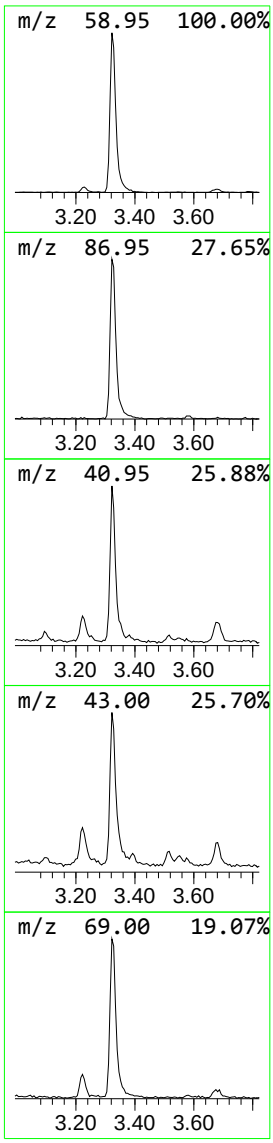
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.322	8.69 ng	270976	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4	Hexanamide	115	C6H13NO	000628-02-4	50
5	Amylene hydrate	88	C5H12O	000075-85-4	42





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Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

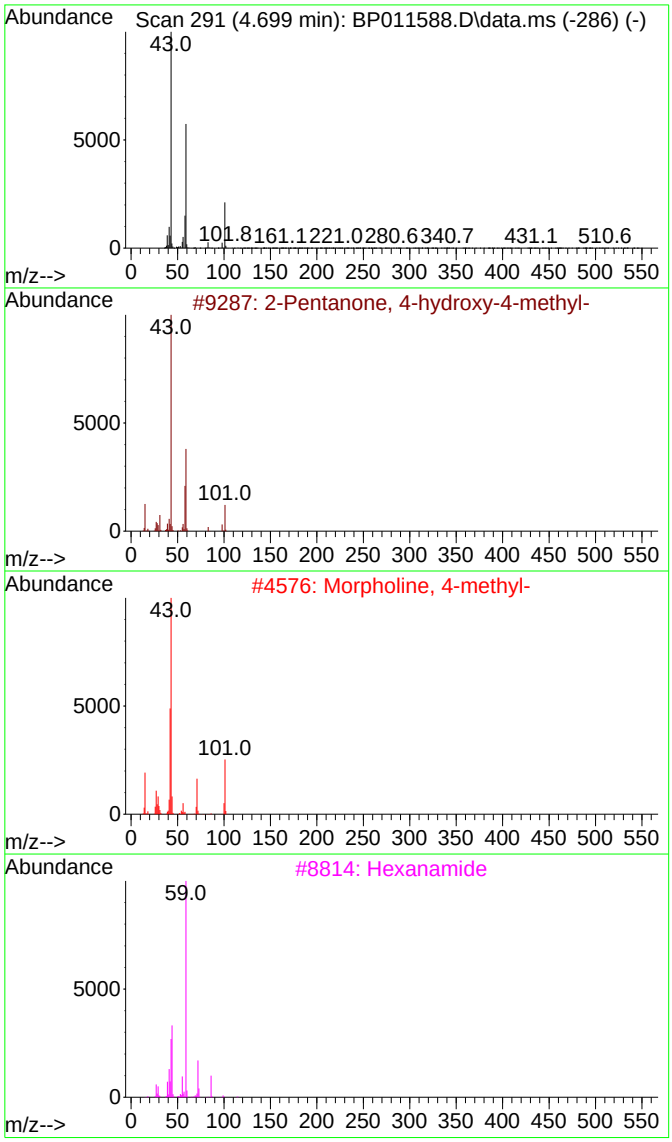
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

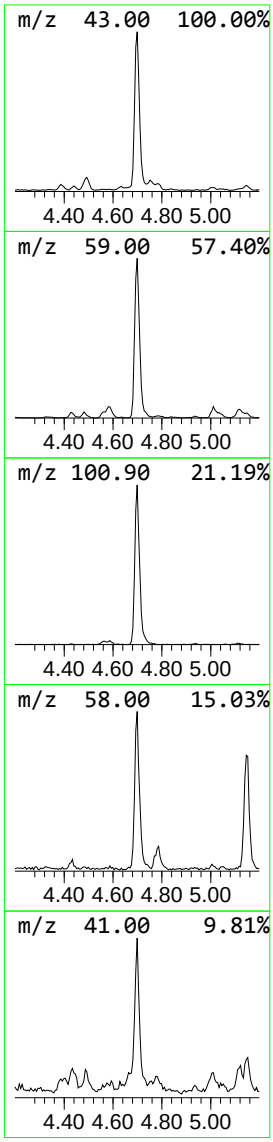
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.699	8.10 ng	252495	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Hexanamide	115	C6H13NO	000628-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





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Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.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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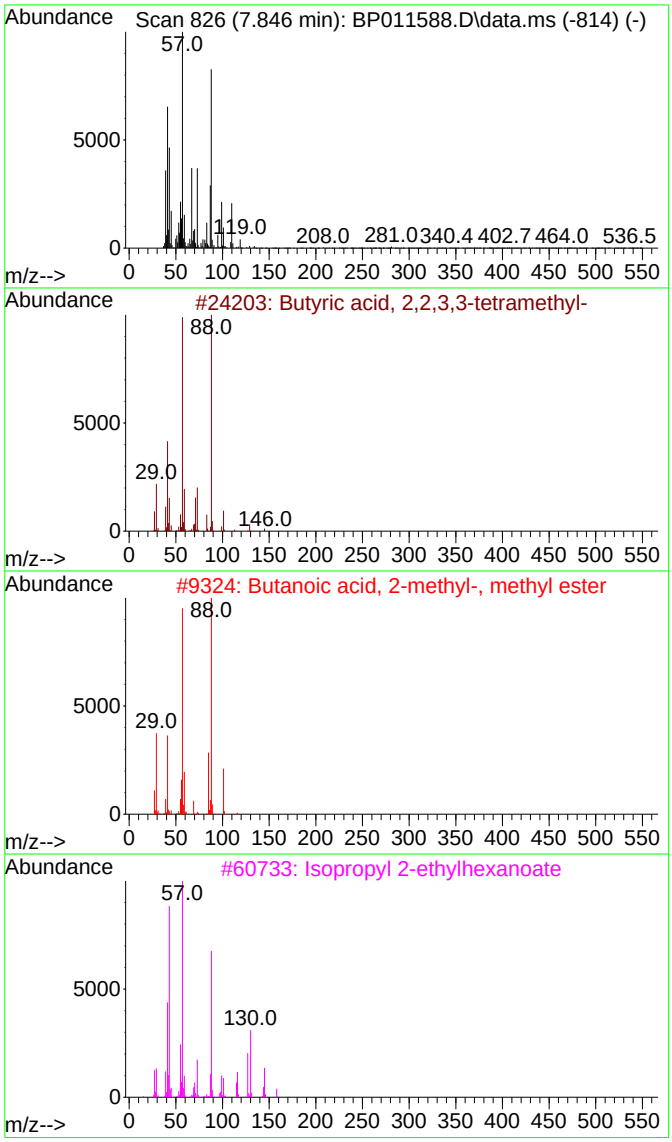
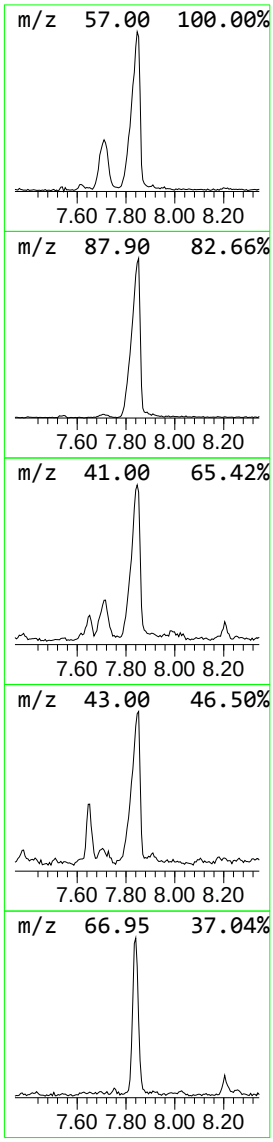
Peak Number 3 unknown7.846 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.846	16.87 ng	525846	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	47
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	43
3	Isopropyl 2-ethylhexanoate	186	C11H22O2	067024-46-8	40
4	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	37
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	35





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Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

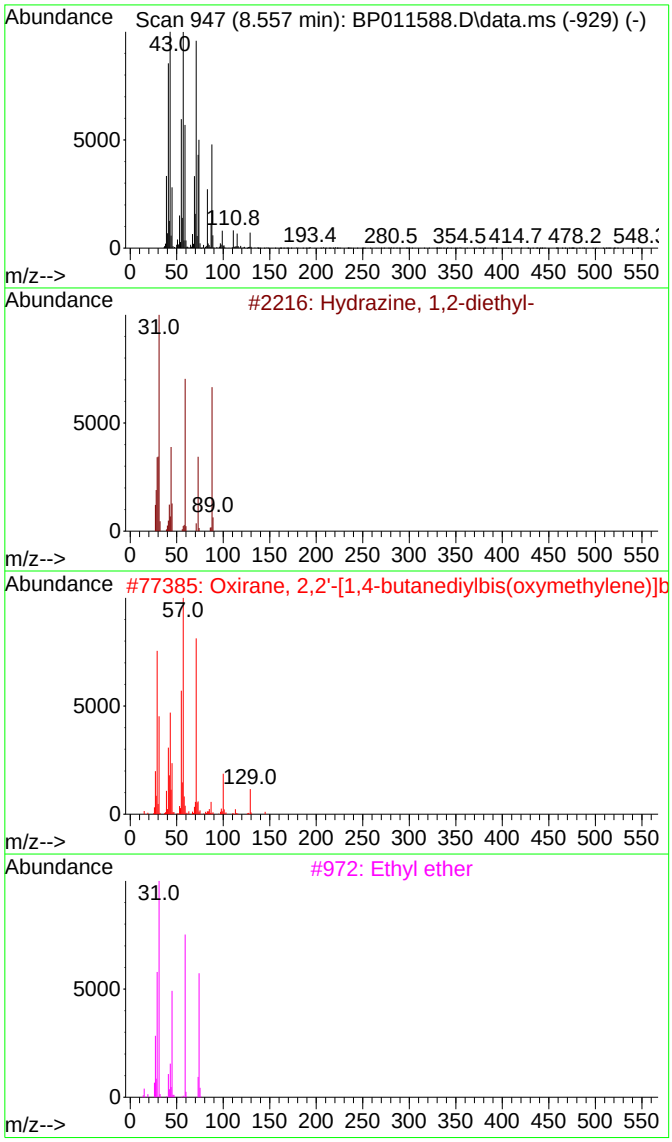
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

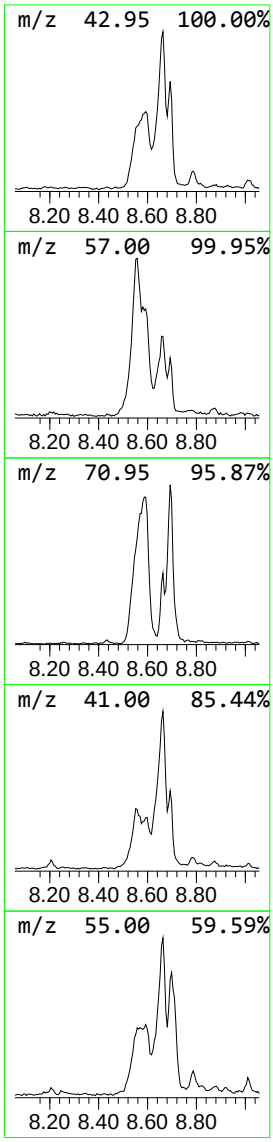
****

Peak Number 4 unknown8.557 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.557	15.79 ng	492302	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	27
2	Oxirane, 2,2'-[1,4-butanediylbis...	202	C10H18O4	002425-79-8	27
3	Ethyl ether	74	C4H10O	000060-29-7	25
4	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	22
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

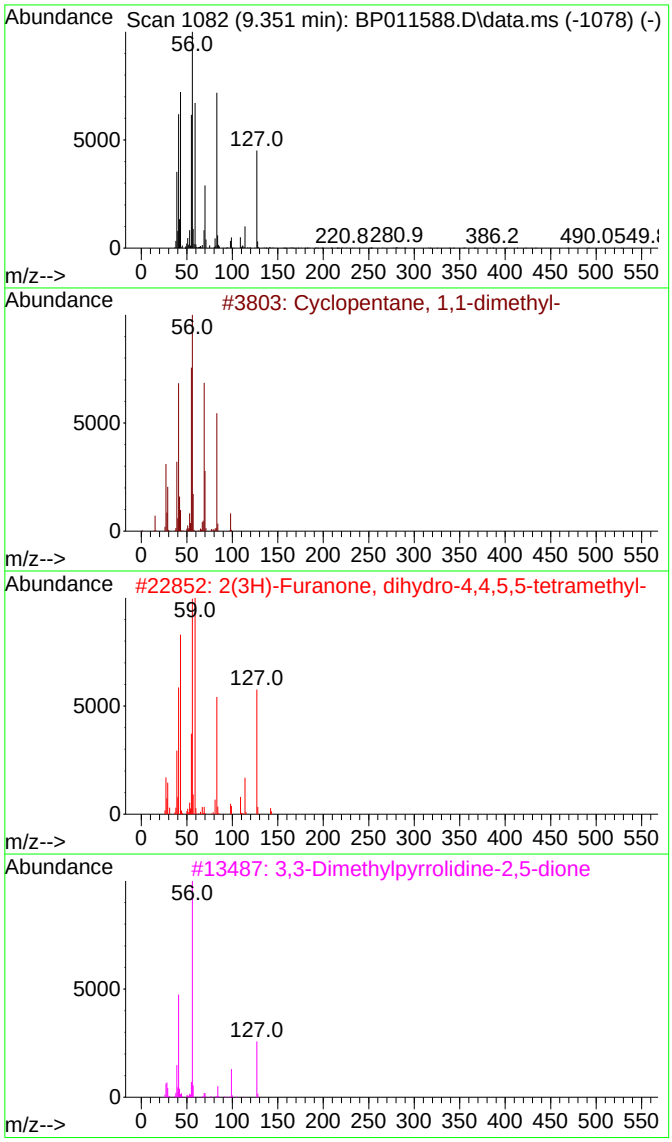
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

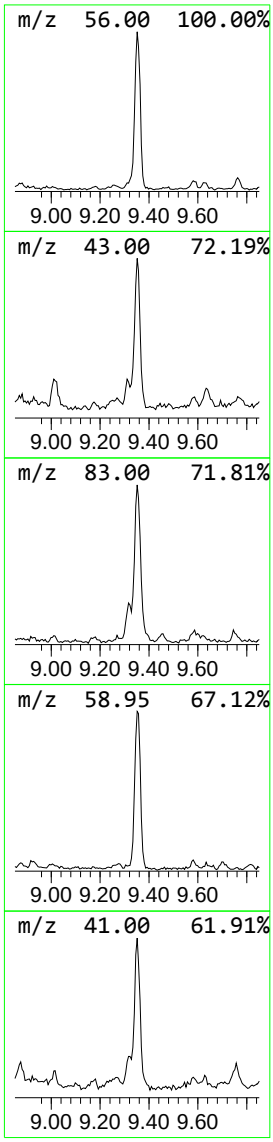
****

Peak Number 5 unknown9.351 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.351	5.02 ng	232051	Naphthalene-d8	10.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	47
2	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	43
3	3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	38
4	2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	35
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
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Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

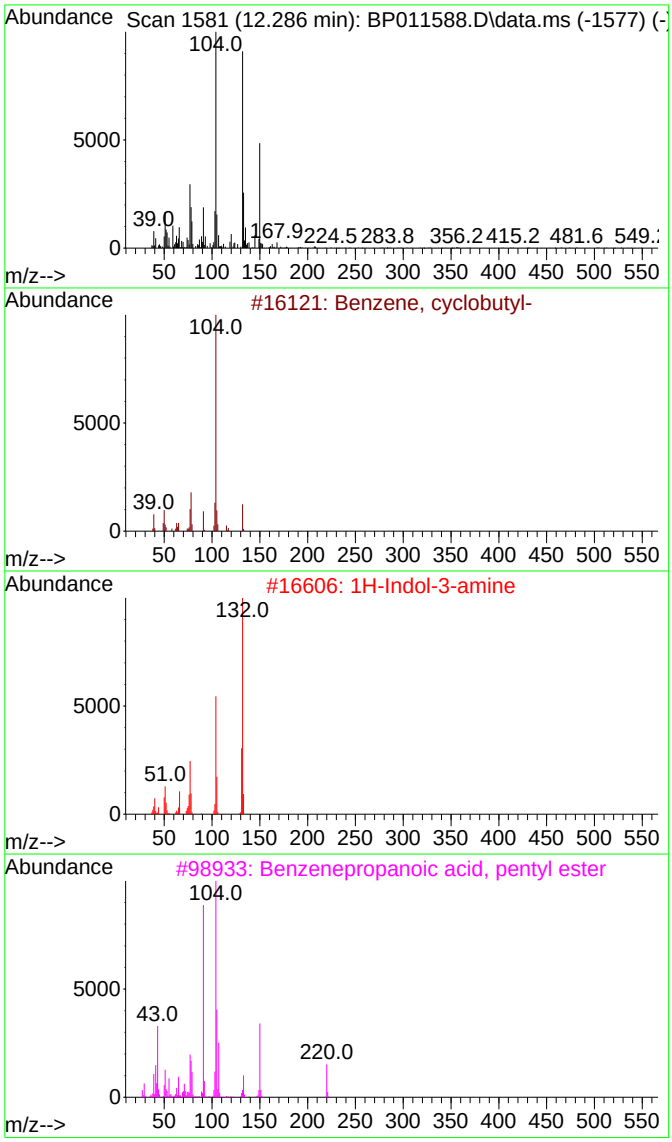
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

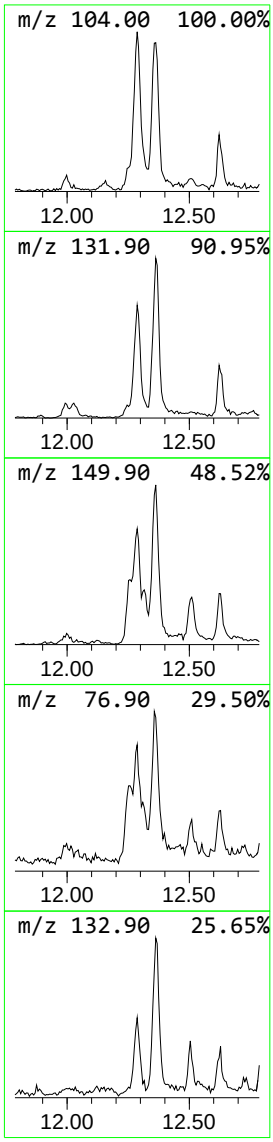
****

Peak Number 6 unknown12.286 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.286	3.43 ng	220767	Acenaphthene-d10	14.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclobutyl-	132	C10H12	004392-30-7	47
2	1H-Indol-3-amine	132	C8H8N2	007250-19-3	46
3	Benzenepropanoic acid, pentyl ester	220	C14H20O2	232949-65-4	43
4	Aziridine, 2-methyl-2-phenyl-	133	C9H11N	022596-57-2	35
5	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
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Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

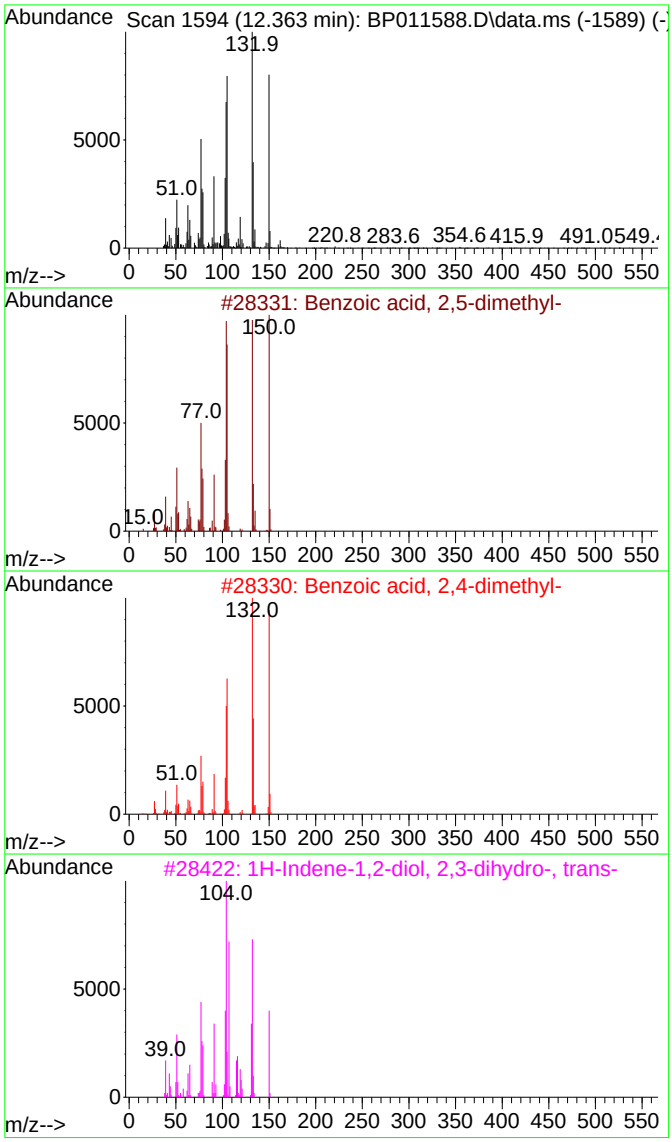
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

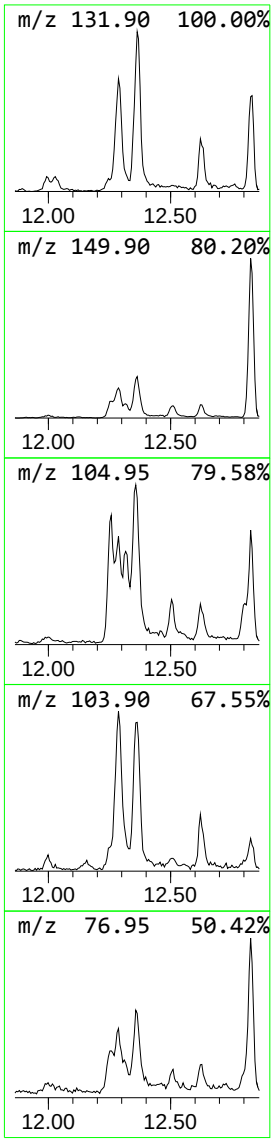
****

Peak Number 7 Benzoic acid, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	3.82 ng	245259	Acenaphthene-d10	14.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	97
2	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	95
3	1H-Indene-1,2-diol, 2,3-dihydro-...	150	C9H10O2	004647-43-2	90
4	Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	90
5	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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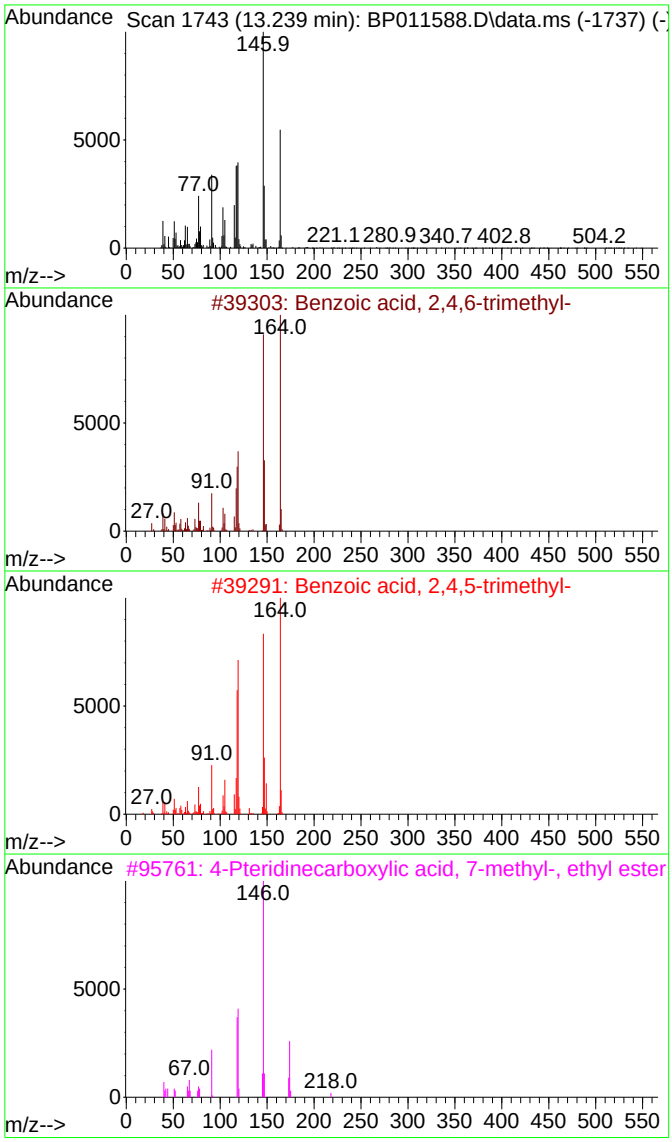
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

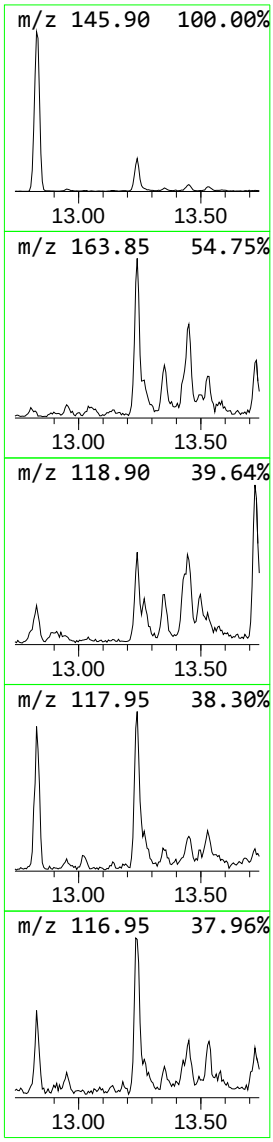
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	2.91 ng	187093	Acenaphthene-d10	14.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	83
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	52
3	4-Pteridinecarboxylic acid, 7-me...	218	C10H10N4O2	016008-52-9	38
4	1,3-Oxazolidine, 4-methyl-2-(4-m...	253	C17H19NO	1000138-83-3	35
5	4-Oxazolecarboxylic acid, 4,5-di...	233	C13H15NO3	037592-54-4	35





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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.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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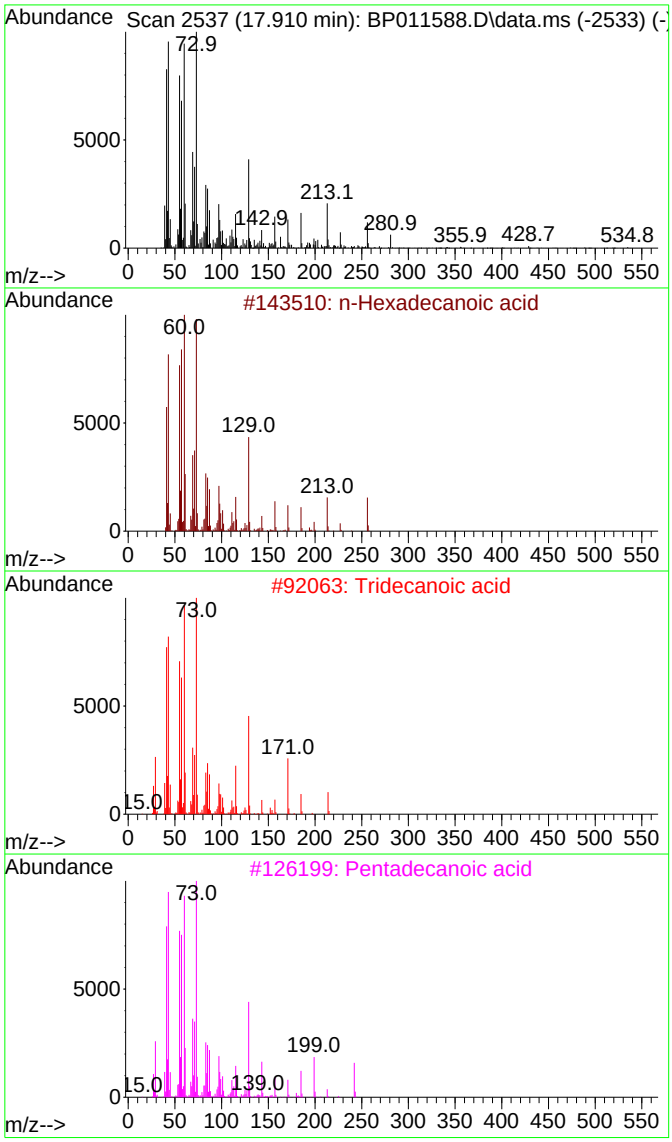
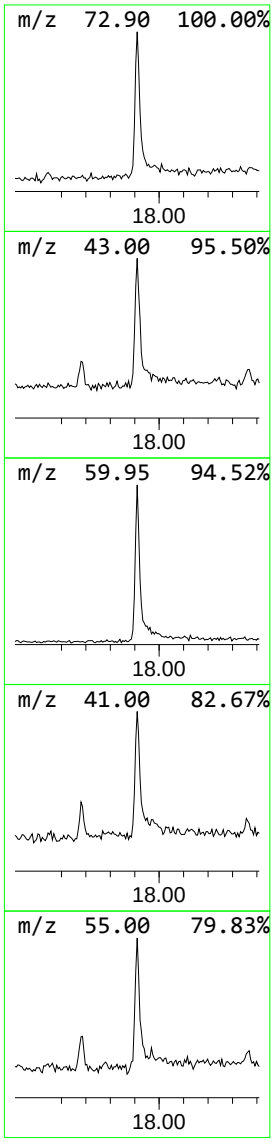
Peak Number 9 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.910	3.33 ng	265286	Phenanthrene-d10	16.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
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Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
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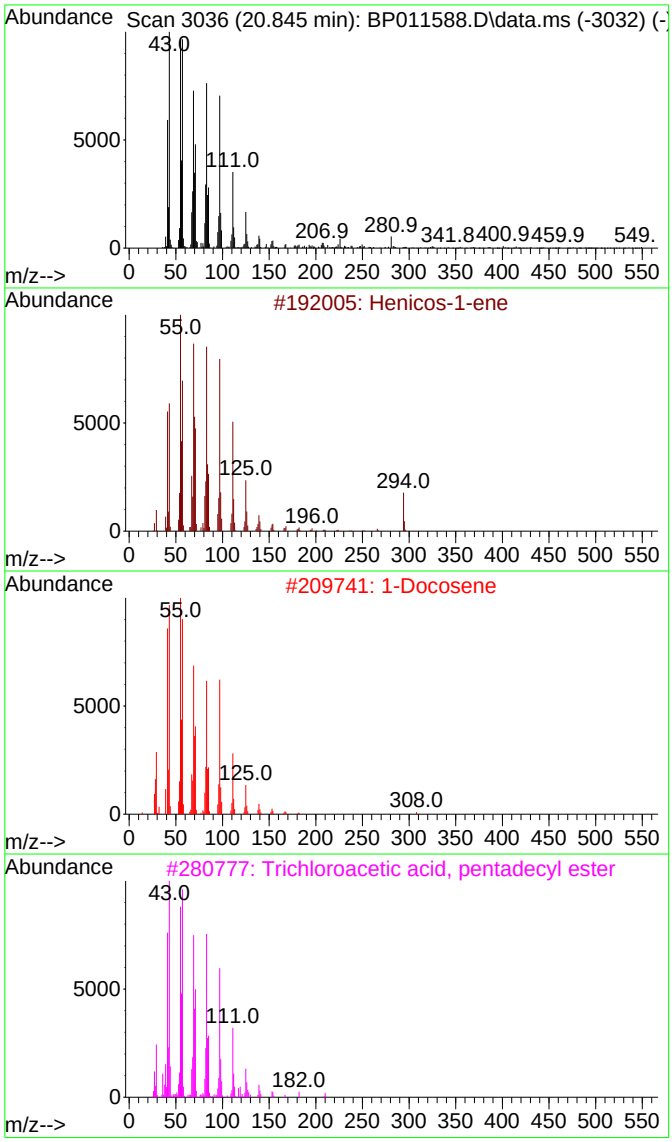
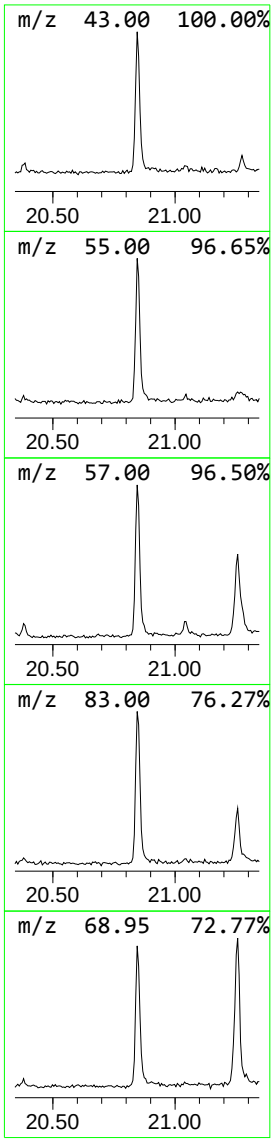
Peak Number 10 Henicos-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	5.36 ng	495423	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Henicos-1-ene	294	C21H42	001599-68-4	97
2	1-Docosene	308	C22H44	001599-67-3	95
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.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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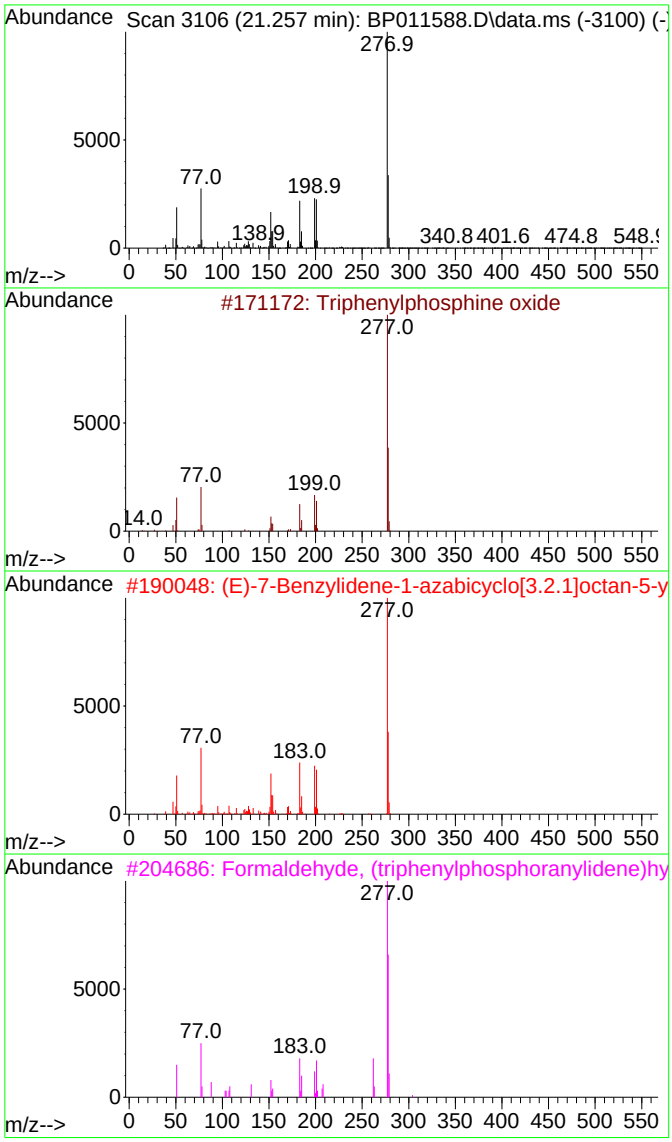
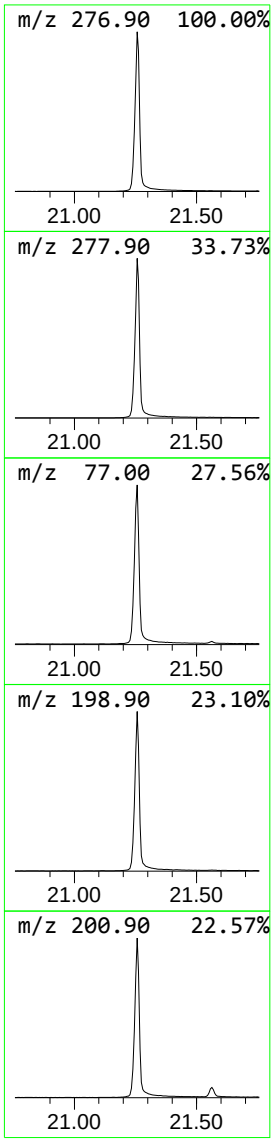
Peak Number 11 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	169.18 ng	15625400	Chrysene-d12	21.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	28
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011588.D
Acq On : 26 Aug 2022 20:23
Operator : CG/JU
Sample : N4355-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.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-Butanol, 2,3-...	3.322	8.7	ng	270976	1	7.540	623485	20.0
2-Pentanone, 4-...	4.699	8.1	ng	252495	1	7.540	623485	20.0
unknown7.846	7.846	16.9	ng	525846	1	7.540	623485	20.0
unknown8.557	8.557	15.8	ng	492302	1	7.540	623485	20.0
unknown9.351	9.351	5.0	ng	232051	2	10.328	924654	20.0
unknown12.286	12.286	3.4	ng	220767	3	14.216	1285720	20.0
Benzoic acid, 2...	12.363	3.8	ng	245259	3	14.216	1285720	20.0
Benzoic acid, 2...	13.239	2.9	ng	187093	3	14.216	1285720	20.0
n-Hexadecanoic ...	17.910	3.3	ng	265286	4	16.986	1591960	20.0
Henicos-1-ene	20.845	5.4	ng	495423	5	21.115	1847220	20.0
Triphenylphosph...	21.257	169.2	ng	15625400	5	21.115	1847220	20.0