LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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: BP011587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.699	286	291	303	rBV	217661	308114	1.86%	0.555%
2	5.069	346	354	361	rVB	107301	167536	1.01%	0.302%
3	5.146	361	367	374	rBV	1227298	1835206	11.06%	3.308%
4	5.222	374	380	387	rVB	143916	257907	1.55%	0.465%
5	6.734	632	637	648	rVB	850168	1358041	8.19%	2.448%
6	6.928	663	670	676	rBV	116514	173414	1.05%	0.313%
7	7.540	767	774	783	rBV	376471	589908	3.56%	1.063%
8	7.646	783	792	801	rVB	95231	167342	1.01%	0.302%
9	7.905	830	836	843	rBV	238907	367807	2.22%	0.663%
10	8.710	966	973	983	rBV	1553771	2479417	14.95%	4.470%
11	9.728	1134	1146	1156	rBV2	114609	236495	1.43%	0.426%
12	10.328	1237	1248	1253	rBV	549112	914549	5.51%	1.649%
13	10.375	1253	1256	1263	rVB	133946	216263	1.30%	0.390%
14	12.234	1565	1572	1578	rBV3	132365	290627	1.75%	0.524%
15	12.828	1665	1673	1679	rBV	3597651	5283240	31.85%	9.524%
16	14.075	1874	1885	1891	rBV	717127	1471955	8.87%	2.653%
17	14.216	1903	1909	1915	rBV	865800	1249321	7.53%	2.252%
18	14.816	1998	2011	2012	rBV4	145121	458007	2.76%	0.826%
19	15.722	2159	2165	2175	rVB	3941185	5285711	31.86%	9.528%
20	16.986	2374	2380	2386	rBV	1110530	1536092	9.26%	2.769%
21	17.916	2534	2538	2543	rBV	167167	244291	1.47%	0.440%
22	19.586	2817	2822	2827	rBV	7902971	9630066	58.05%	17.360%
23	20.845	3032	3036	3043	rBV	312052	447945	2.70%	0.807%
24	21.116	3077	3082	3086	rBV	1507687	1852046	11.16%	3.339%
25	21.257	3099	3106	3136	rBV	12661198	16589904	100.00%	29.906%
26	23.398	3464	3470	3484	rVB2	1070172	2062555	12.43%	3.718%

Sum of corrected areas: 55473759

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
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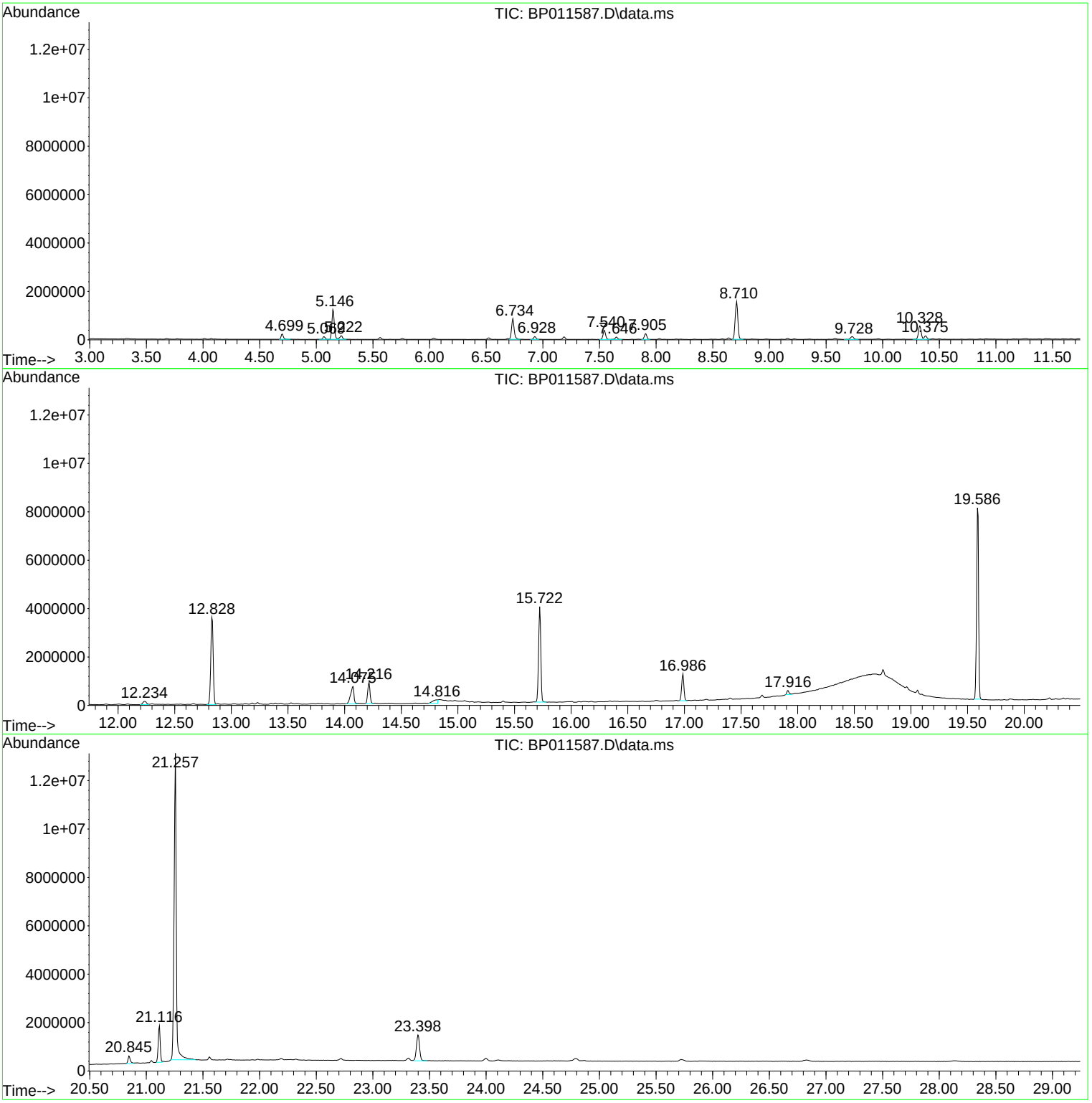
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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 : BP011587.D
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Instrument :
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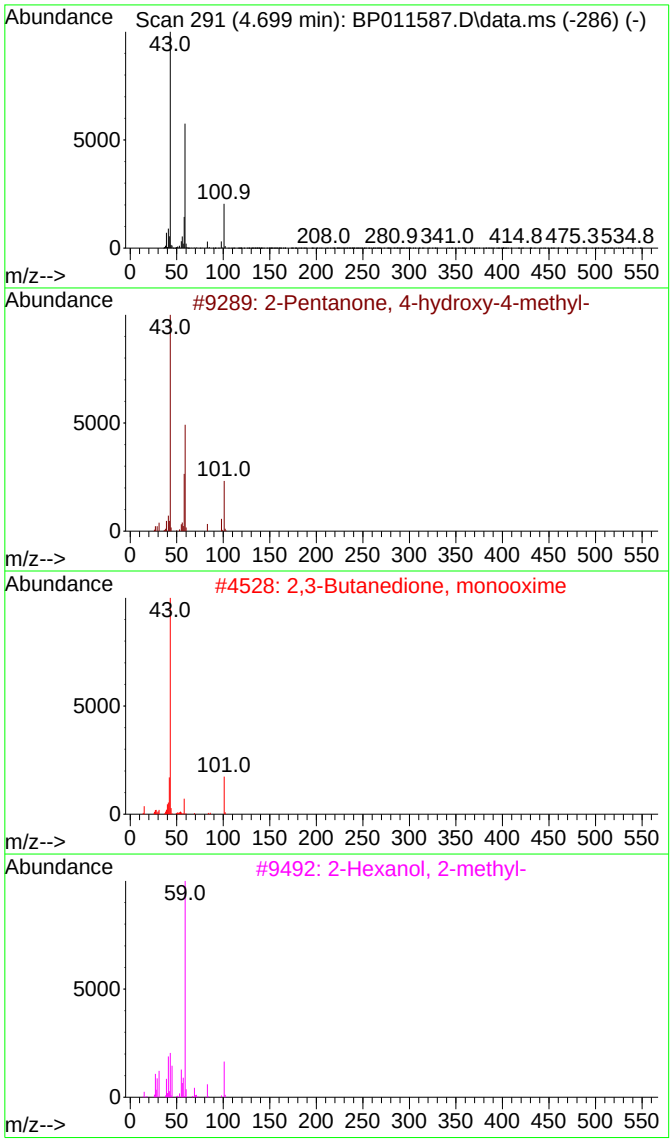
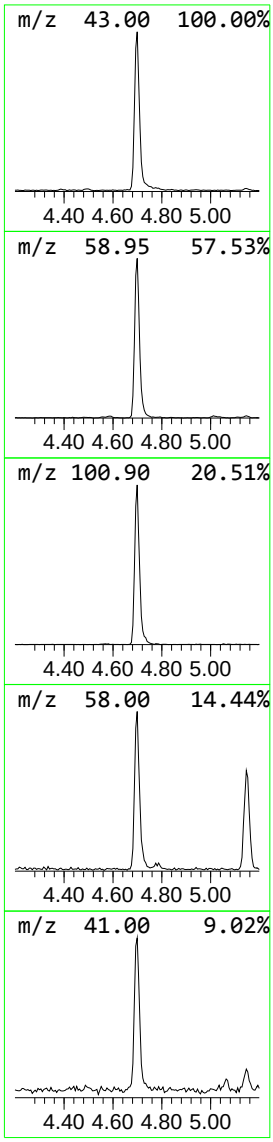
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.699	10.45 ng	308114	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	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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

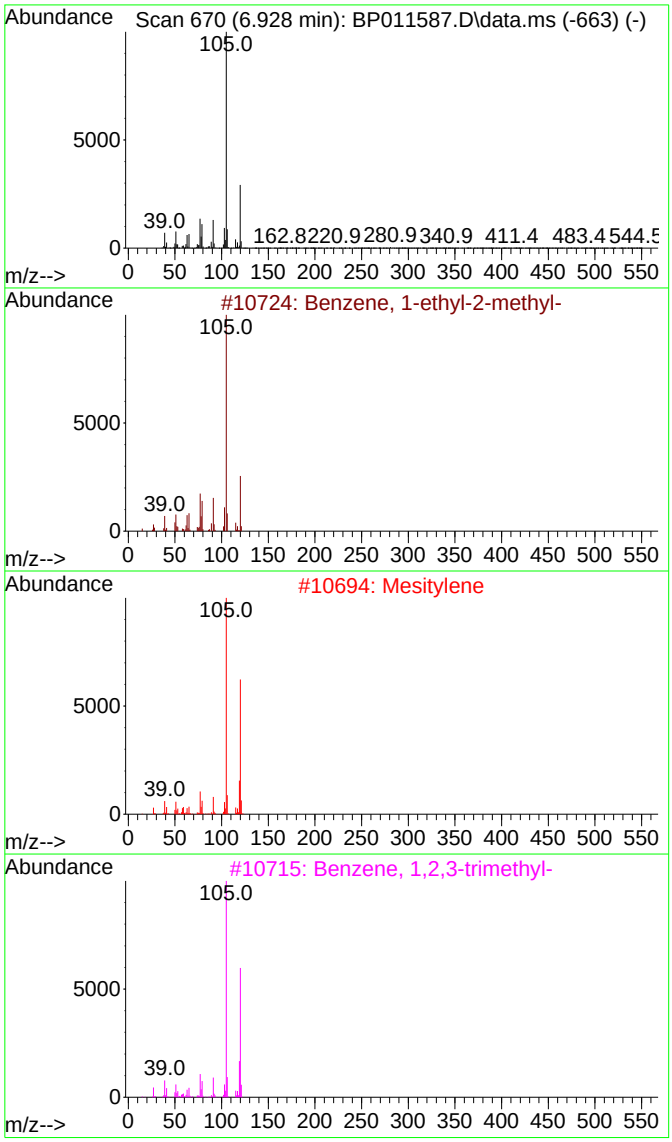
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

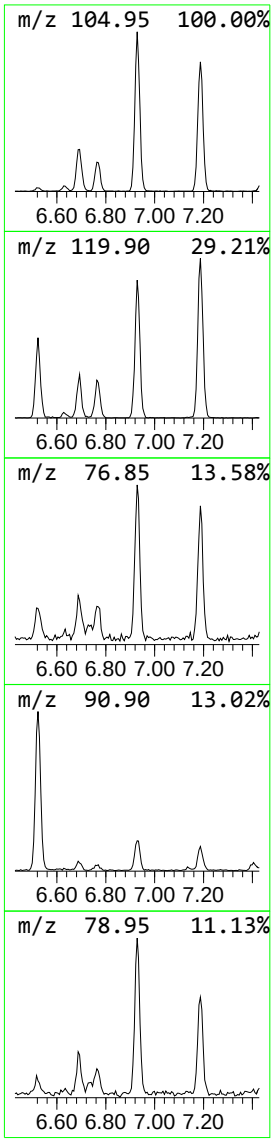
****

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	5.88 ng	173414	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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

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TIC Integration Parameters: LSCINT.P

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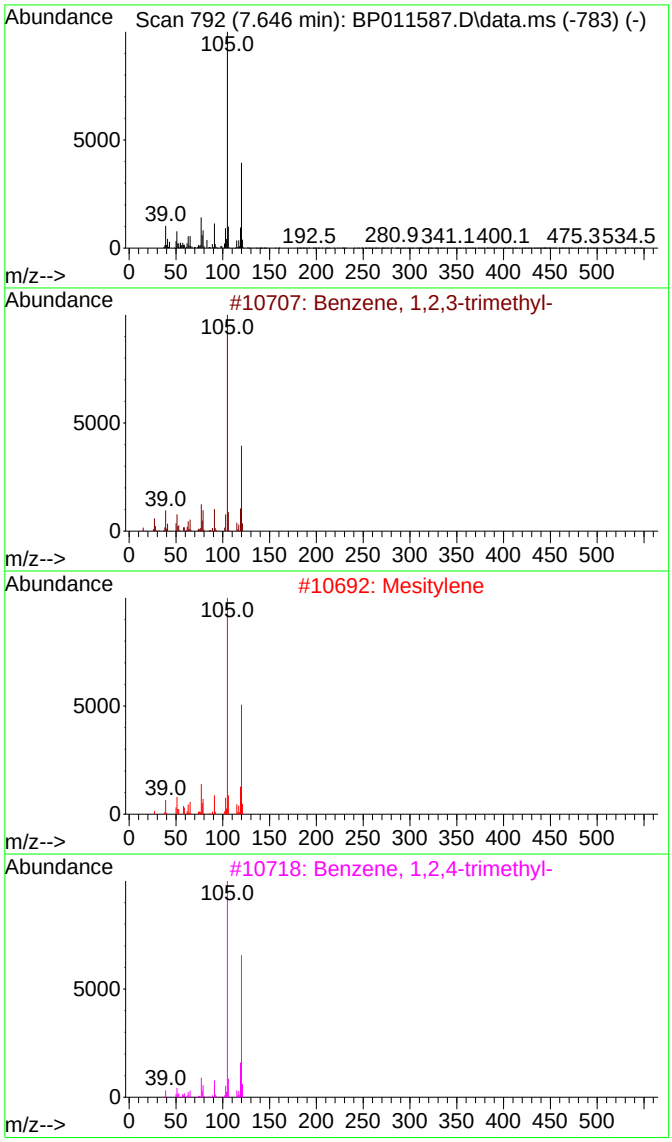
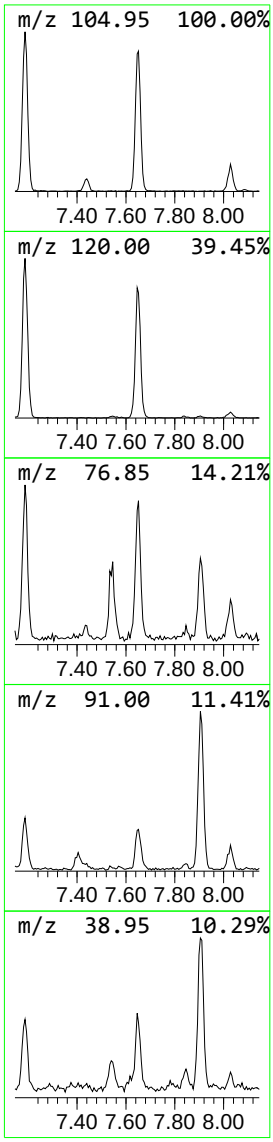
Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.646	5.67 ng	167342	1,4-Dichlorobenzene-d4	7.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Mesitylene	120	C9H12	000108-67-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
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Sample : N4355-01
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
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
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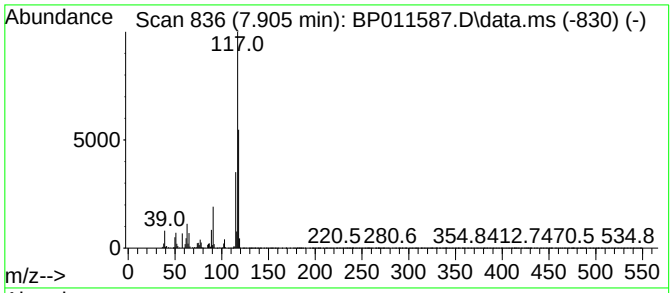
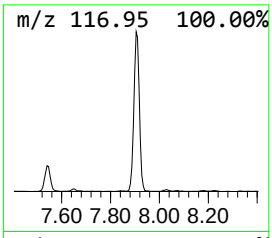
****

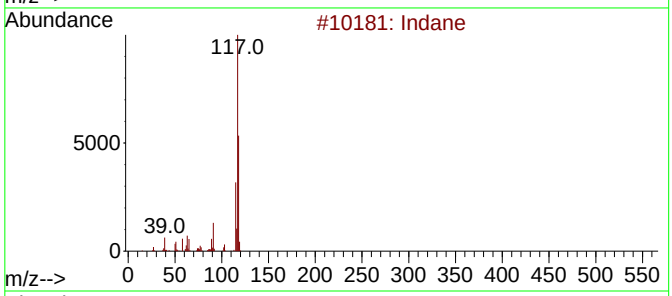
Peak Number 6 Indane Concentration Rank 3

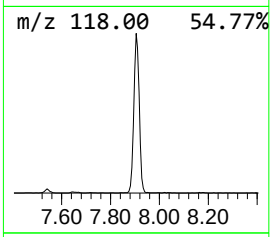
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.905	12.47 ng	367807	1,4-Dichlorobenzene-d4	7.540

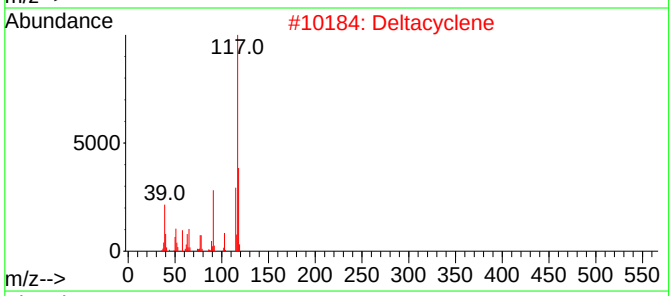
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Deltacyclene	118	C9H10	007785-10-6	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5	Indole	117	C8H7N	000120-72-9	50

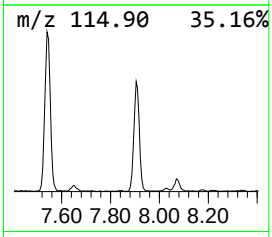


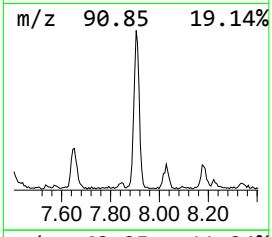


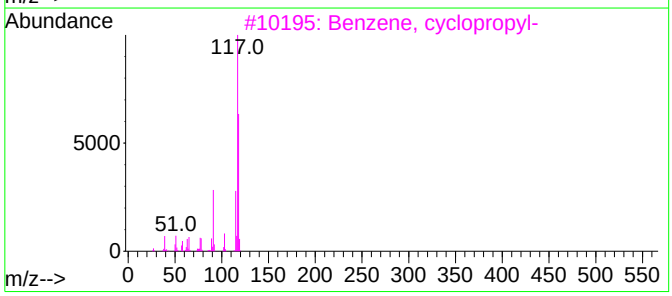


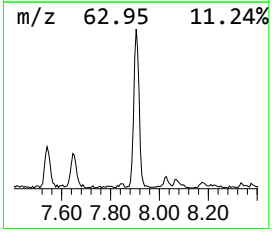












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
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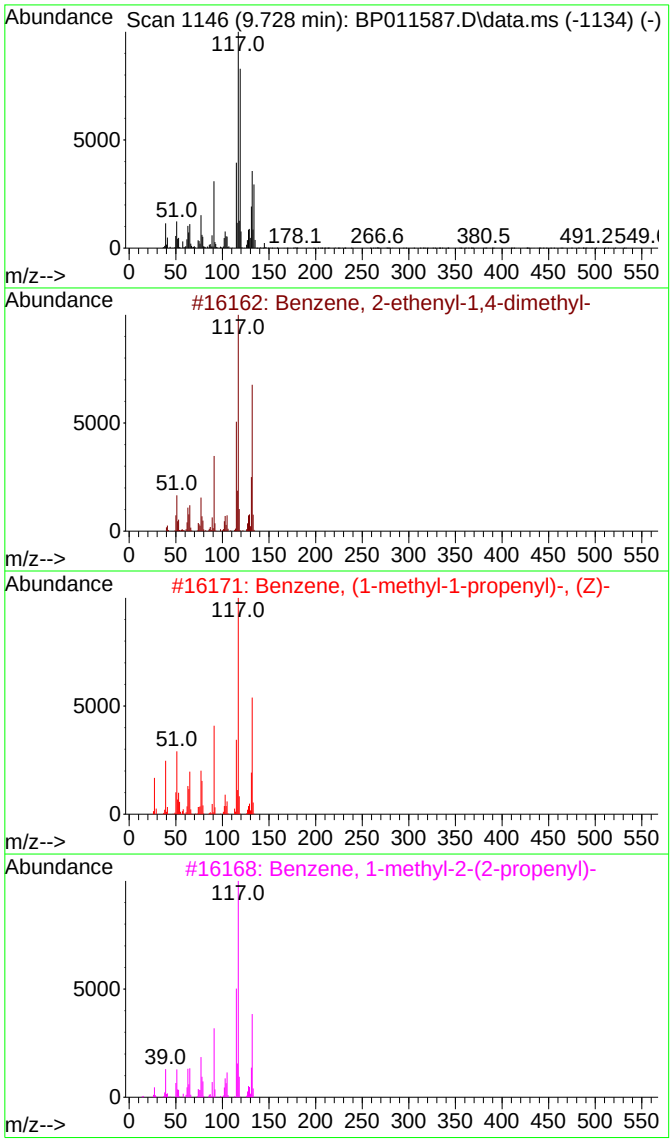
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP082622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

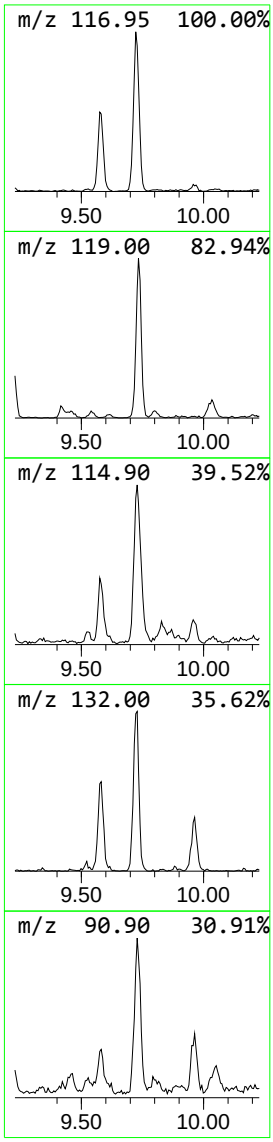
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	5.17 ng	236495	Naphthalene-d8	10.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	83
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	60
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	60
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	60
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	55





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

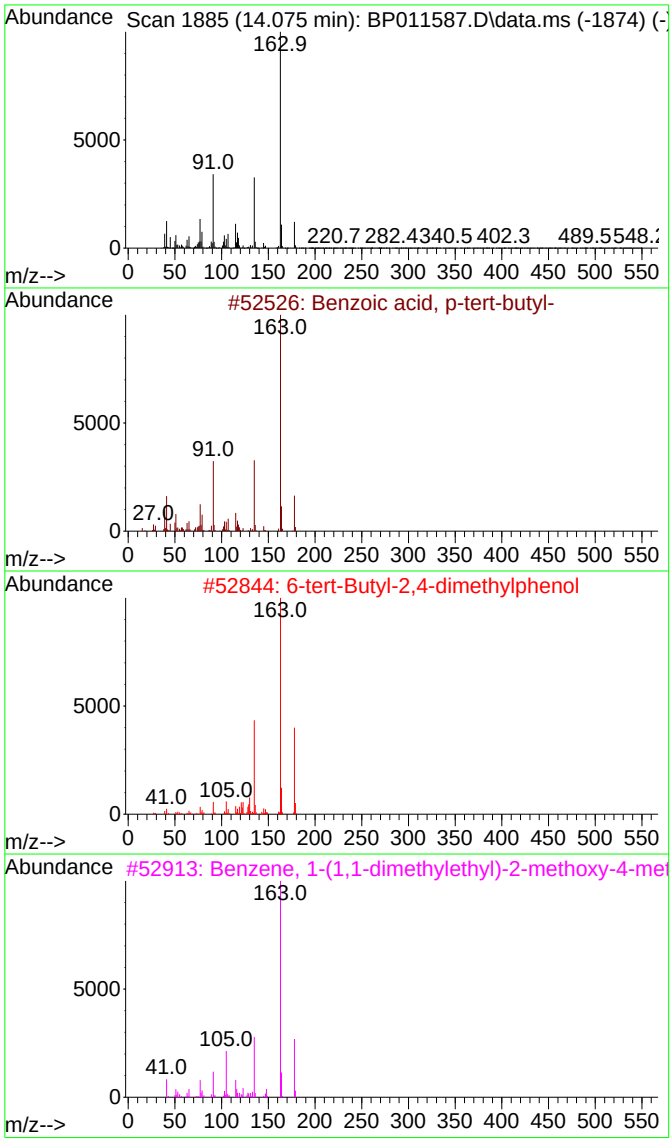
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

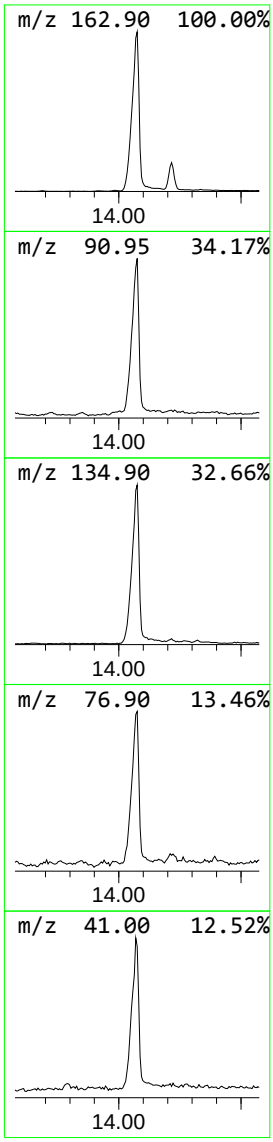
****

Peak Number 8 Benzoic acid, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	23.56 ng	1471960	Acenaphthene-d10	14.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	95
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	68
3	Benzene, 1-(1,1-dimethylethyl)-2...	178	C12H18O	000088-40-4	59
4	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	59
5	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	50





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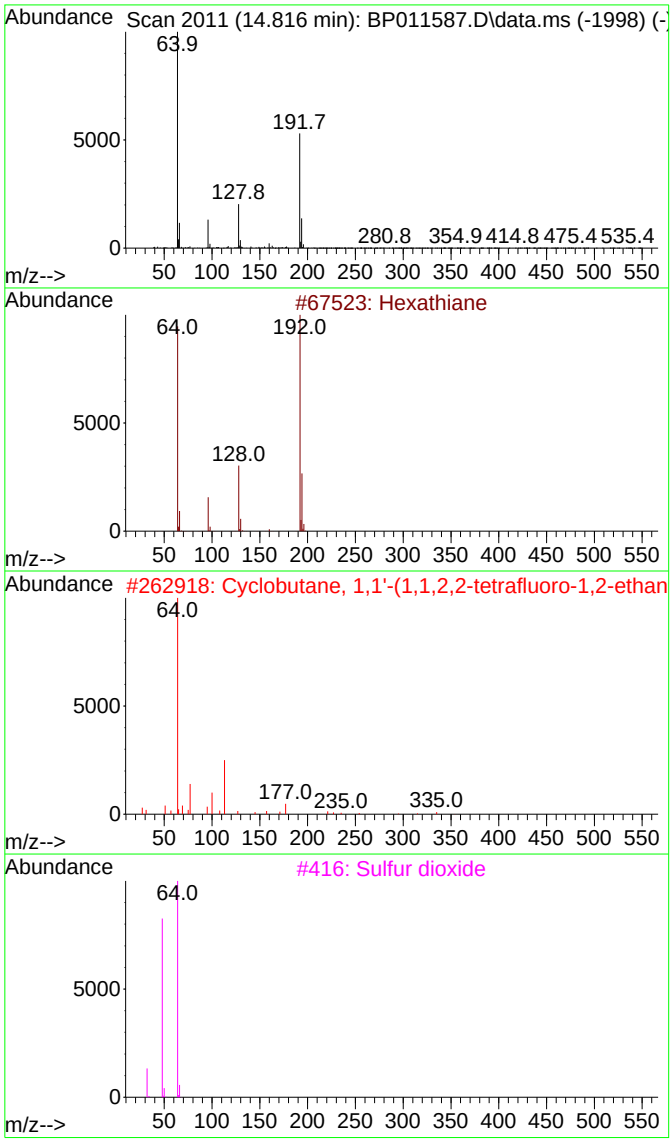
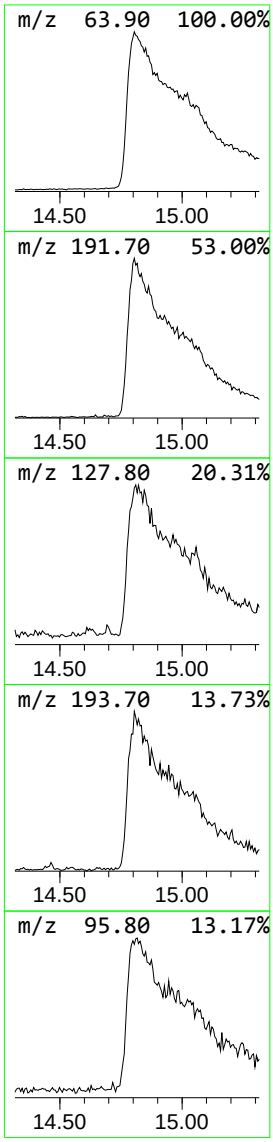
****

Peak Number 9 Hexathiane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	7.33 ng	458007	Acenaphthene-d10	14.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Cyclobutane, 1,1'-(1,1,2,2-tetra...	354	C10H6F12	035207-94-4	5
3	Sulfur dioxide	64	O2S	007446-09-5	4
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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BNA_P
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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
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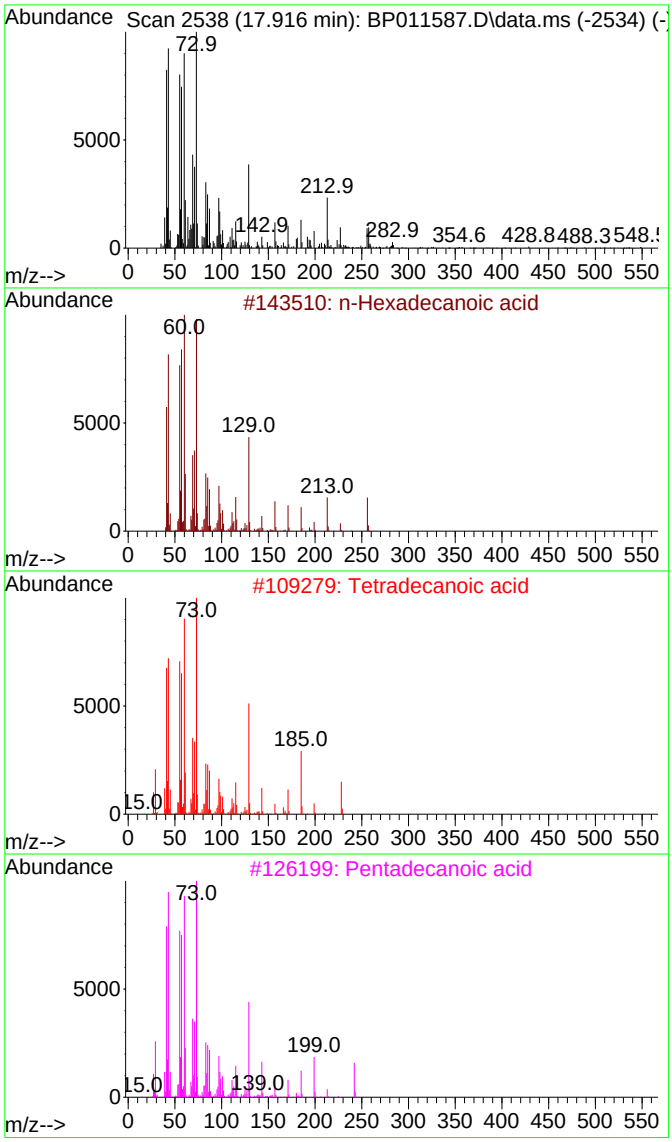
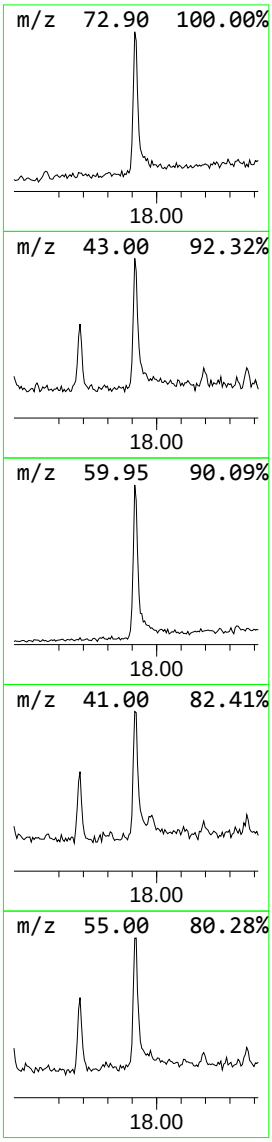
Peak Number 10 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.916	3.18 ng	244291	Phenanthrene-d10	16.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





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Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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

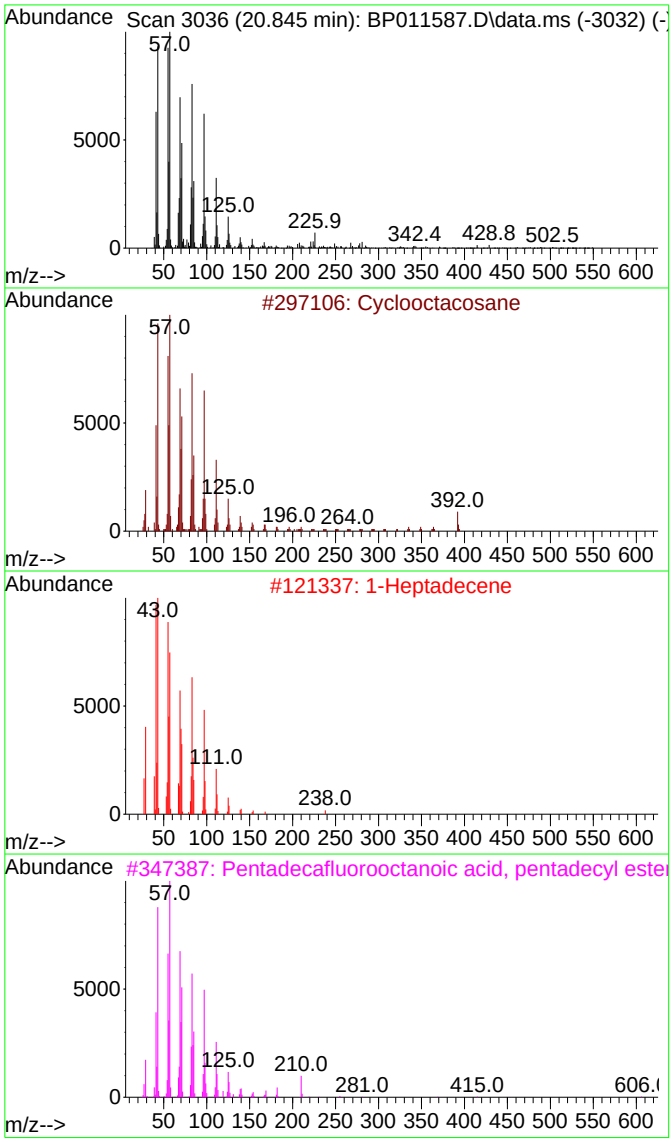
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

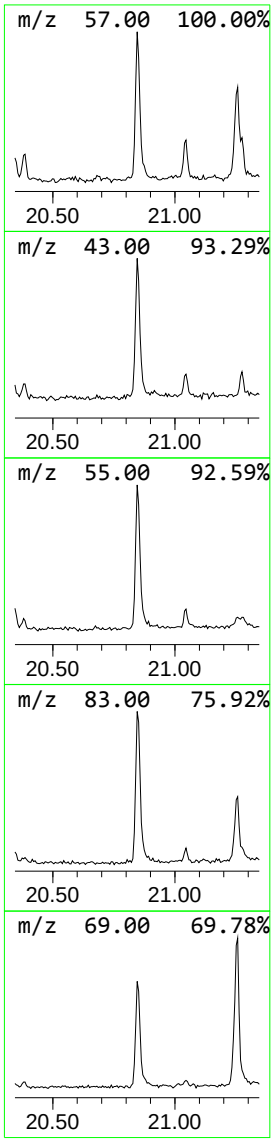
****

Peak Number 11 Cyclooctacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	4.84 ng	447945	Chrysene-d12	21.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctacosane	392	C28H56	000297-24-5	98
2	1-Heptadecene	238	C17H34	006765-39-5	95
3	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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

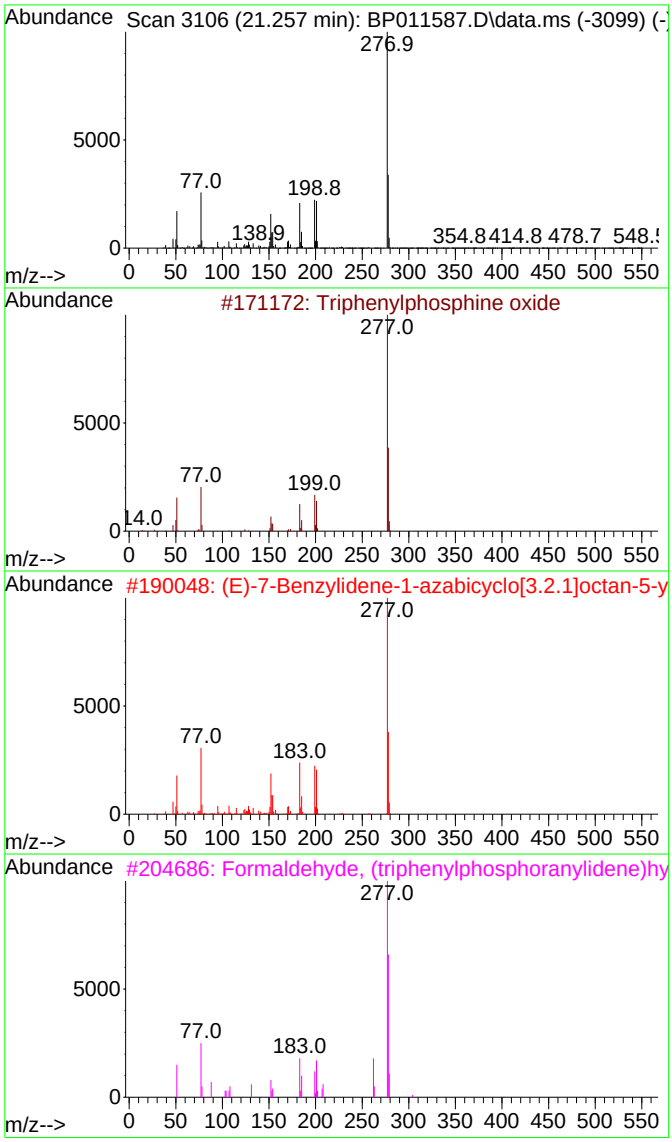
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

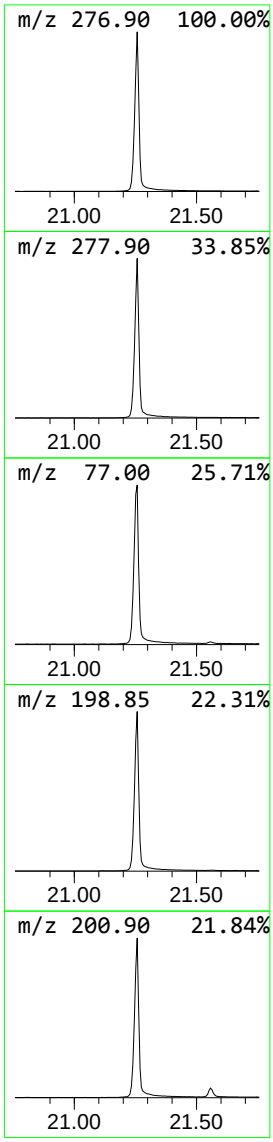
****

Peak Number 12 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	179.15 ng	16589900	Chrysene-d12	21.116

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	50
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082622\
Data File : BP011587.D
Acq On : 26 Aug 2022 19:48
Operator : CG/JU
Sample : N4355-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-31

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-Pentanone, 4-...	4.699	10.4	ng	308114	1	7.540	589908	20.0
Benzene, 1-ethy...	6.928	5.9	ng	173414	1	7.540	589908	20.0
Benzene, 1,2,3-...	7.646	5.7	ng	167342	1	7.540	589908	20.0
Indane	7.905	12.5	ng	367807	1	7.540	589908	20.0
Benzene, 2-ethe...	9.728	5.2	ng	236495	2	10.328	914549	20.0
Benzoic acid, p...	14.075	23.6	ng	1471960	3	14.216	1249320	20.0
Hexathiane	14.816	7.3	ng	458007	3	14.216	1249320	20.0
n-Hexadecanoic ...	17.916	3.2	ng	244291	4	16.986	1536090	20.0
Cyclooctacosane	20.845	4.8	ng	447945	5	21.116	1852050	20.0
Triphenylphosph...	21.257	179.2	ng	16589900	5	21.116	1852050	20.0