LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011827.D
Acq On : 27 Sep 2022 21:49
Operator : CG/JU
Sample : N4815-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-2

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-BP092122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	6	10	29	rVB	2226073	3341723	17.25%	2.855%
2	5.005	337	343	356	rVB	426330	673479	3.48%	0.575%
3	5.470	415	422	438	rBV	5791448	8879035	45.83%	7.586%
4	7.069	686	694	715	rBV	5795873	9634653	49.73%	8.232%
5	7.905	829	836	844	rBV	1360946	2237195	11.55%	1.911%
6	9.075	1026	1035	1052	rBV	3467757	5766899	29.77%	4.927%
7	10.499	1272	1277	1295	rBV	135902	319417	1.65%	0.273%
8	10.716	1306	1314	1326	rBV	1988425	3469260	17.91%	2.964%
9	13.175	1724	1732	1746	rBV	9106597	13794638	71.20%	11.786%
10	13.446	1771	1778	1787	rBV	147067	248785	1.28%	0.213%
11	14.551	1959	1966	1976	rBV	3177442	4704412	24.28%	4.019%
12	16.045	2213	2220	2240	rBV	7227690	10600859	54.72%	9.057%
13	17.310	2428	2435	2440	rBV	3740184	5569276	28.75%	4.758%
14	18.192	2580	2585	2609	rBV	1019488	2037310	10.52%	1.741%
15	19.104	2736	2740	2745	rBV	295267	319794	1.65%	0.273%
16	19.310	2772	2775	2782	rBV	124424	225093	1.16%	0.192%
17	19.422	2789	2794	2809	rBV	2105214	3736107	19.28%	3.192%
18	19.681	2833	2838	2852	rBV	4919744	6672753	34.44%	5.701%
19	19.863	2863	2869	2878	rBV	15289632	19374477	100.00%	16.553%
20	21.098	3075	3079	3087	rBV	1269694	2059207	10.63%	1.759%
21	21.392	3123	3129	3134	rBV	4462324	6120170	31.59%	5.229%
22	21.510	3146	3149	3162	rBV	890621	1292289	6.67%	1.104%
23	23.827	3537	3543	3555	rVB2	2970567	5965345	30.79%	5.097%

Sum of corrected areas: 117042176

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ClientSampleId :
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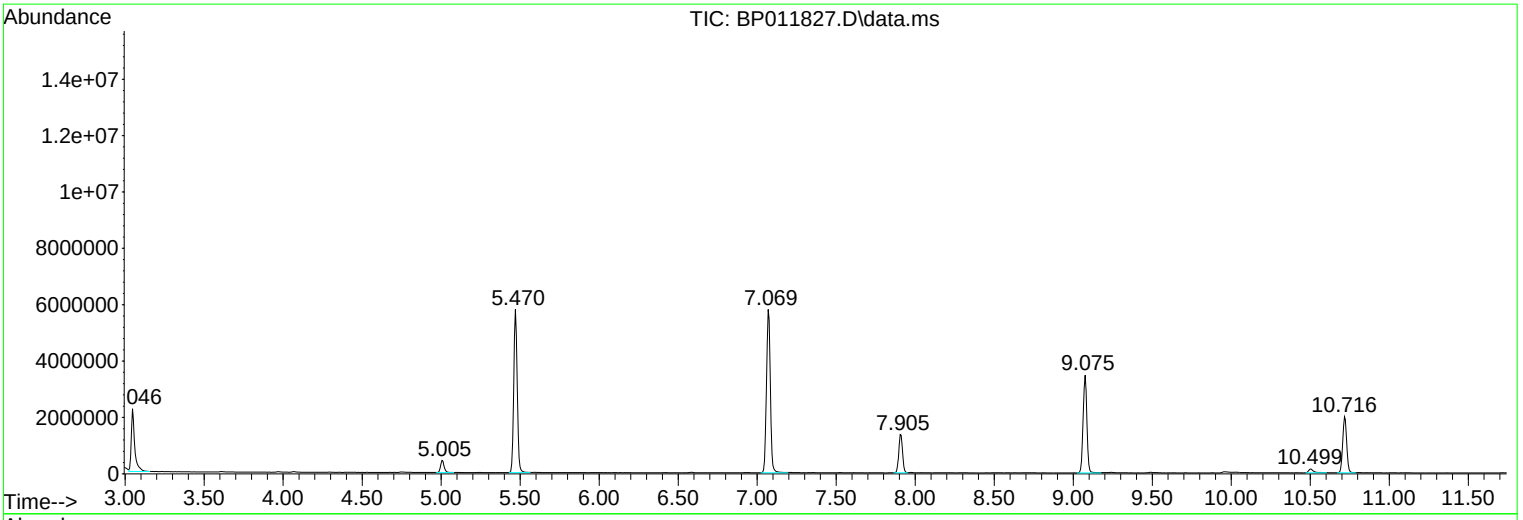
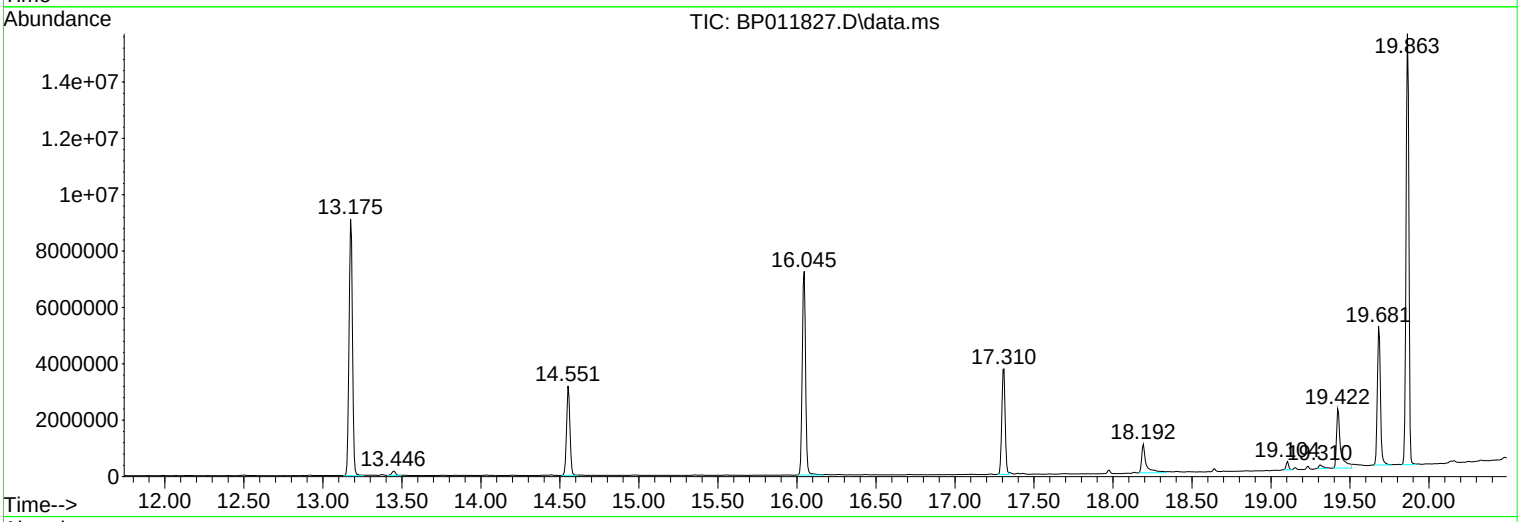
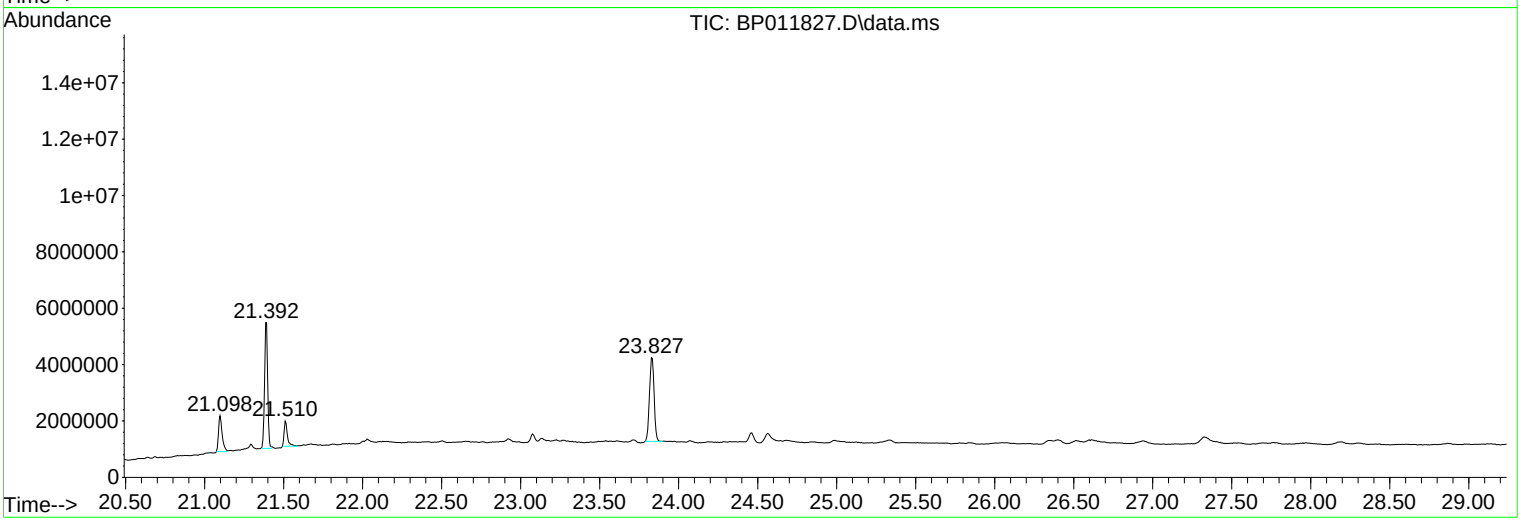
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BP011827.D
Acq On : 27 Sep 2022 21:49
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

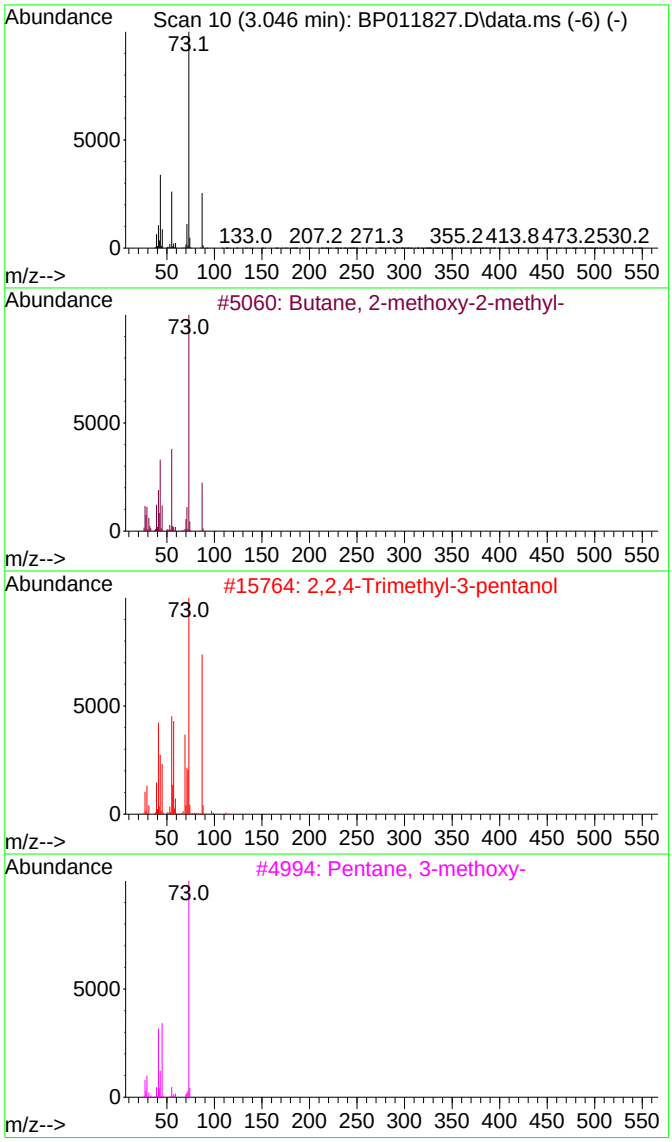
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

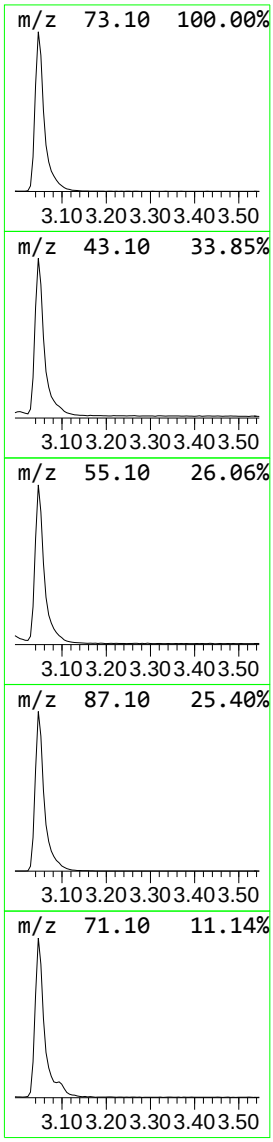
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	29.87 ng	3341720	1,4-Dichlorobenzene-d4	7.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BP011827.D
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Operator : CG/JU
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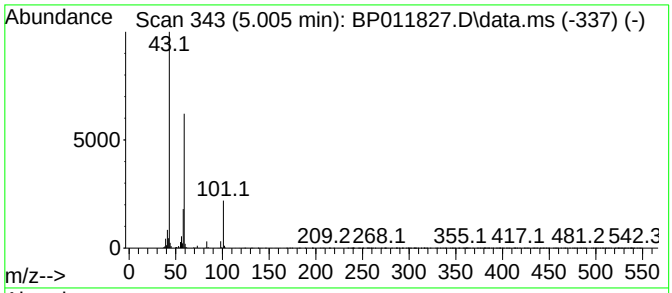
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

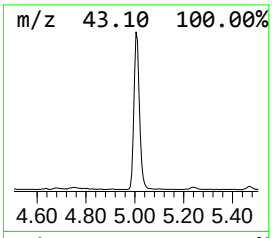
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

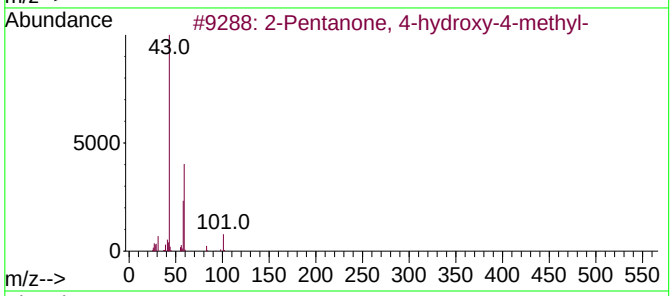
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

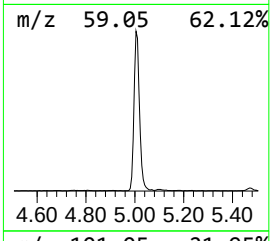
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.005	6.02 ng	673479	1,4-Dichlorobenzene-d4	7.905

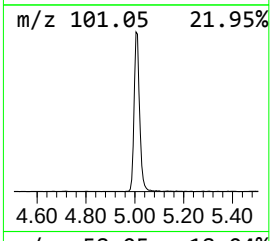
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

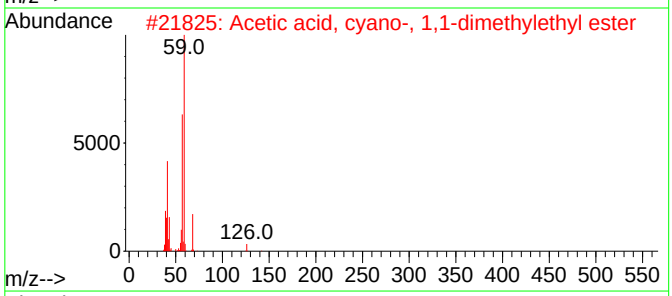


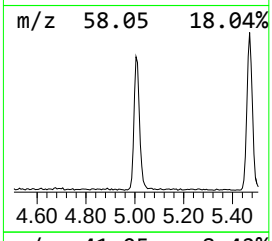


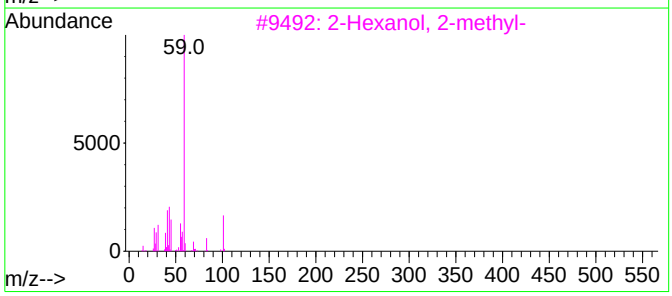


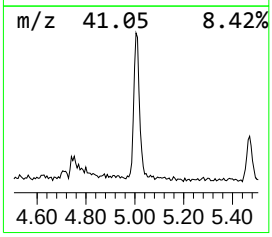












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011827.D
Acq On : 27 Sep 2022 21:49
Operator : CG/JU
Sample : N4815-02
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Instrument :
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ClientSampleId :
SAND-FILTER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

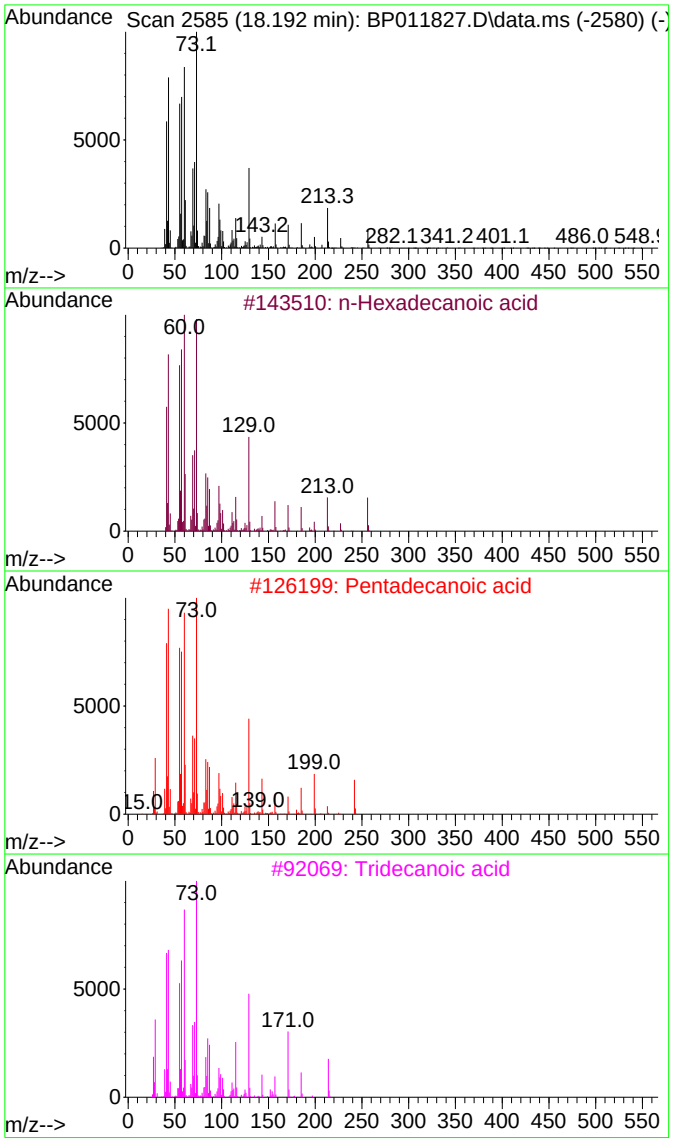
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

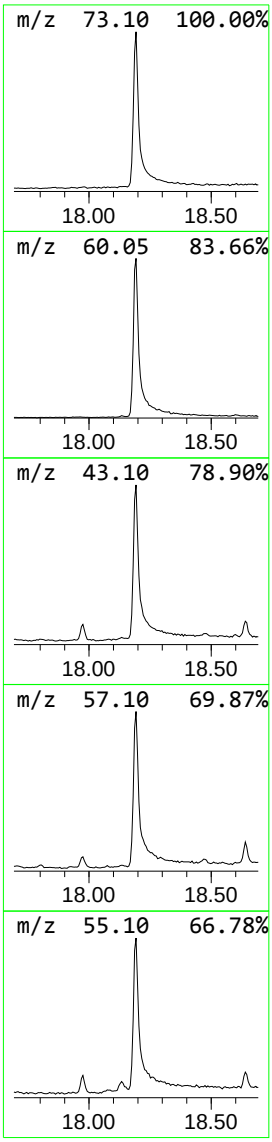
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	7.32 ng	2037310	Phenanthrene-d10	17.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





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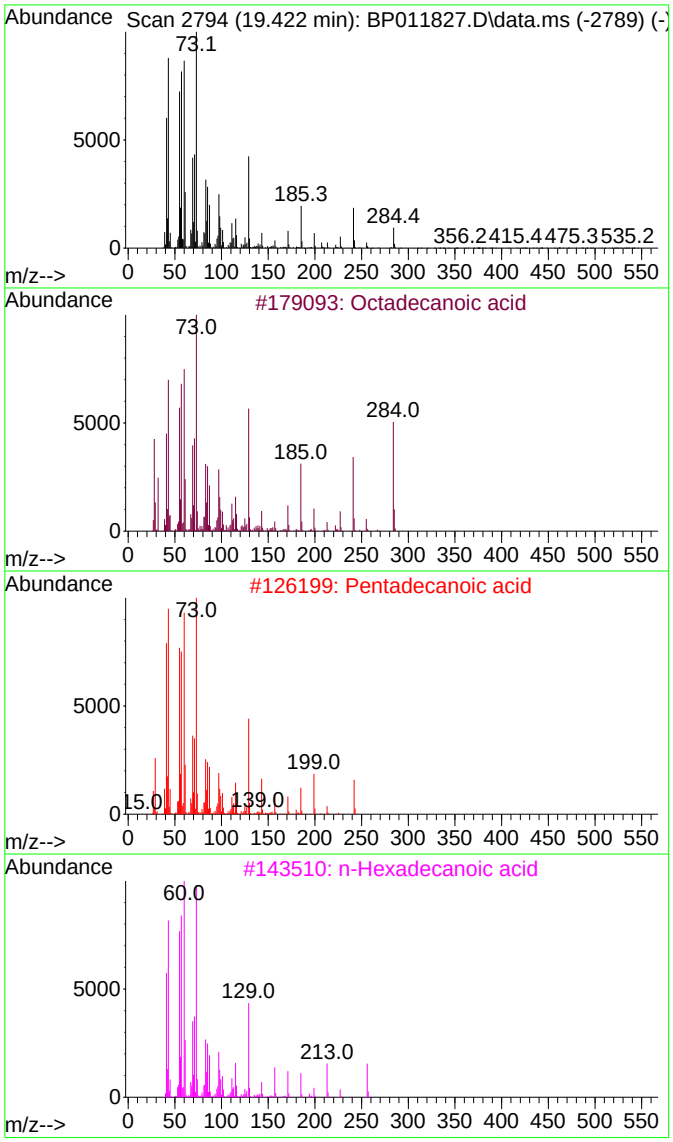
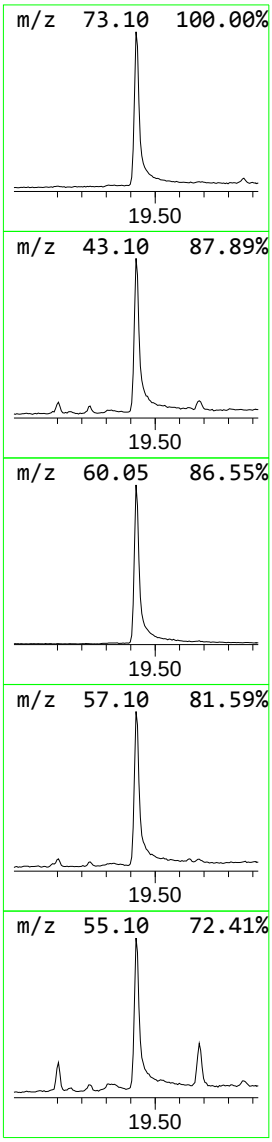
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	12.21 ng	3736110	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87





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Sample : N4815-02
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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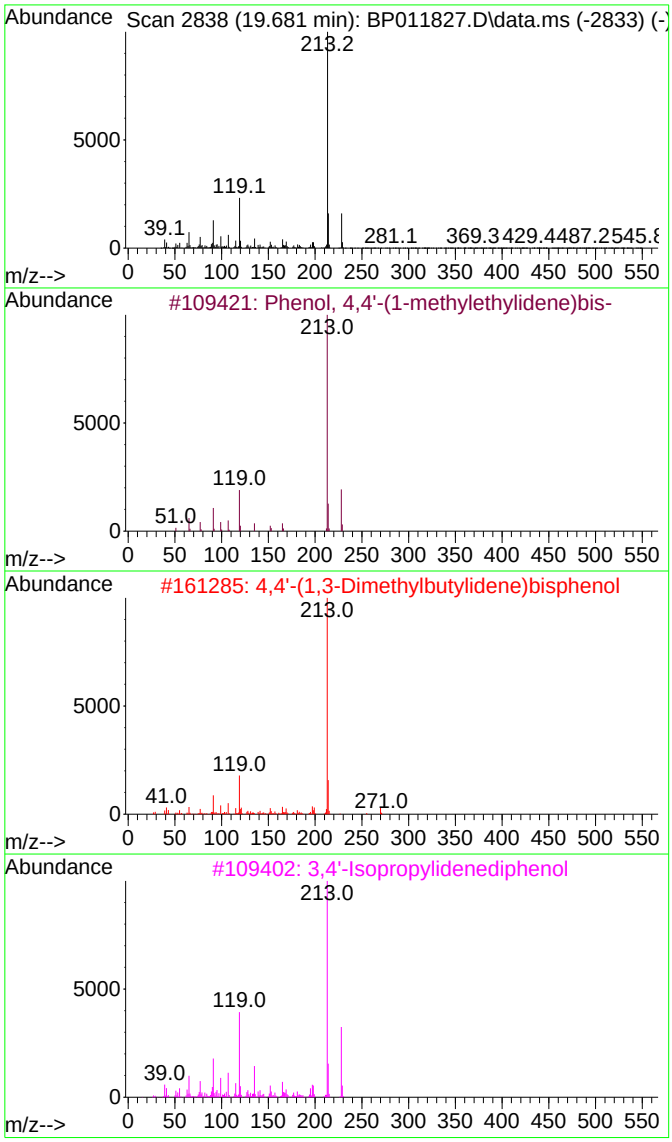
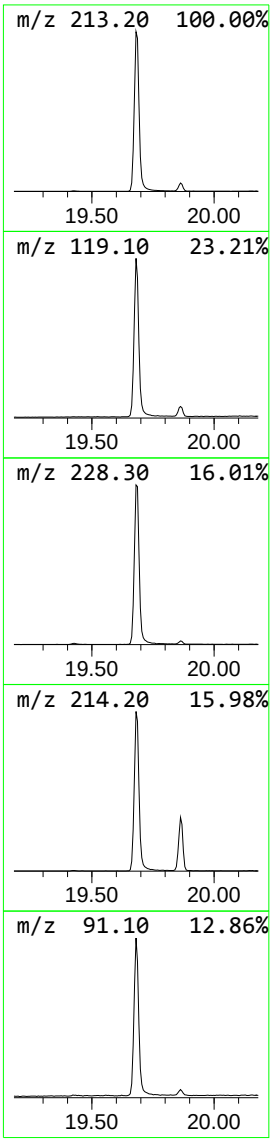
****
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.680	21.81 ng	6672750	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	74
3	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	60
4	Diphenolic acid	286	C17H18O4	000126-00-1	56
5	5-Fluoro-2-nitrophenylamine, TMS...	228	C9H13FN2O2Si	1000484-54-5	53





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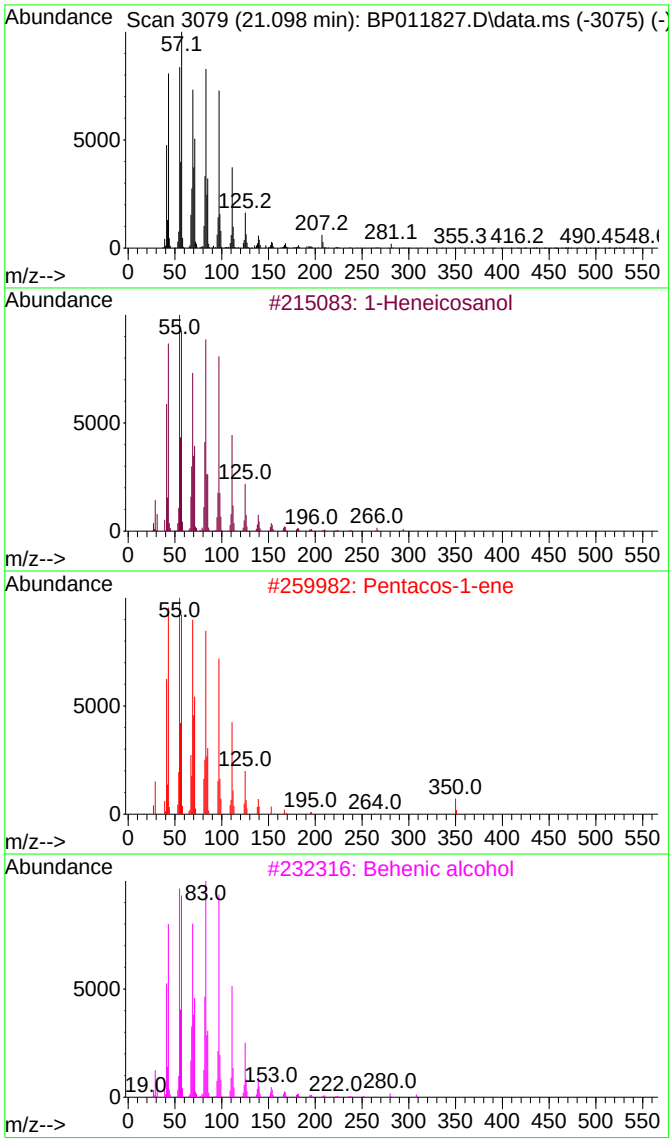
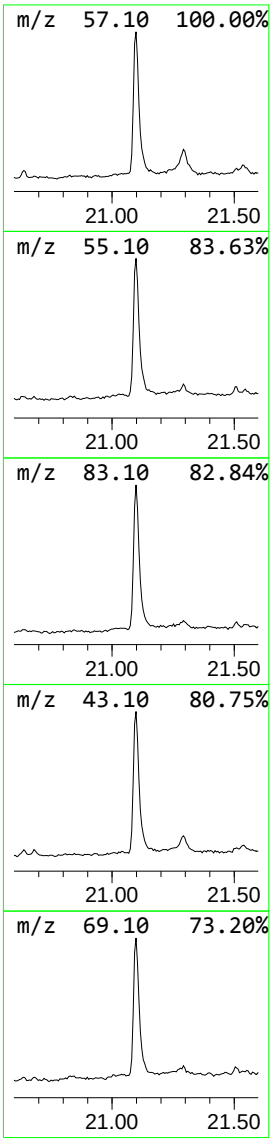
****

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	6.73 ng	2059210	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	1-Heptadecene	238	C17H34	006765-39-5	93





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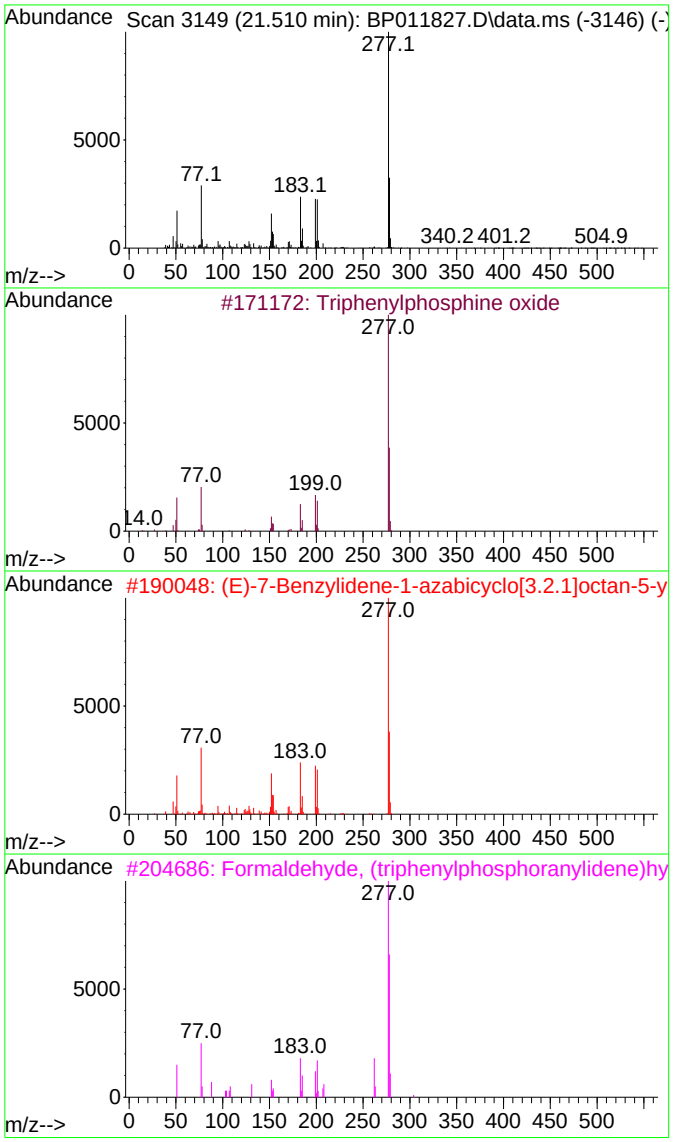
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

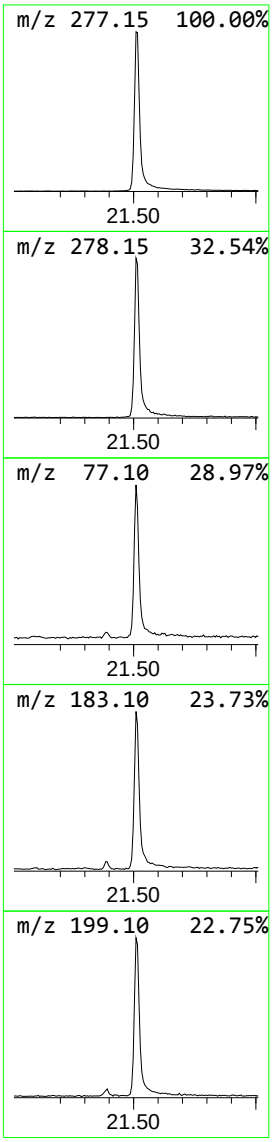
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.510	4.22 ng	1292290	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	95
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011827.D
Acq On : 27 Sep 2022 21:49
Operator : CG/JU
Sample : N4815-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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...	3.046	29.9	ng	3341720	1	7.905	2237200	20.0
2-Pentanone, 4-...	5.005	6.0	ng	673479	1	7.905	2237200	20.0
n-Hexadecanoic ...	18.192	7.3	ng	2037310	4	17.310	5569280	20.0
Octadecanoic acid	19.422	12.2	ng	3736110	5	21.392	6120170	20.0
Phenol, 4,4'-(1...	19.680	21.8	ng	6672750	5	21.392	6120170	20.0
1-Heneicosanol	21.098	6.7	ng	2059210	5	21.392	6120170	20.0
Triphenylphosph...	21.510	4.2	ng	1292290	5	21.392	6120170	20.0