

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
 Data File : BP009057.D
 Acq On : 08 Feb 2022 14:24
 Operator : CG/JU
 Sample : N1397-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 KTS1-MH-01-0-15

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-BP020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009057.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	403	409	426	rBV	1624717	2661884	7.02%	3.075%
2	6.987	671	680	703	rBV	1433532	2647984	6.98%	3.059%
3	7.805	809	819	828	rBV	526392	872873	2.30%	1.008%
4	8.963	1009	1016	1038	rBV	964596	1791952	4.72%	2.070%
5	10.604	1287	1295	1310	rBV	667995	1245094	3.28%	1.438%
6	13.069	1707	1714	1730	rBV	2865897	4269114	11.26%	4.932%
7	14.445	1942	1948	1957	rBV	948143	1482178	3.91%	1.712%
8	15.945	2197	2203	2223	rBV	2050357	3165358	8.35%	3.657%
9	17.204	2411	2417	2423	rBV	1167836	1752399	4.62%	2.025%
10	18.104	2566	2570	2584	rBV2	300806	522396	1.38%	0.604%
11	19.339	2776	2780	2789	rBV	221003	393442	1.04%	0.455%
12	19.769	2848	2853	2860	rBV	4306487	5575815	14.70%	6.442%
13	21.057	3060	3072	3073	rBV2	2281226	6345387	16.73%	7.331%
14	21.122	3074	3083	3104	rVB2	8291941	37924987	100.00%	43.815%
15	21.304	3109	3114	3118	rBV	1601374	2108584	5.56%	2.436%
16	21.416	3128	3133	3140	rBV	7799886	11144196	29.38%	12.875%
17	23.704	3516	3522	3533	rVB2	1333268	2652894	7.00%	3.065%

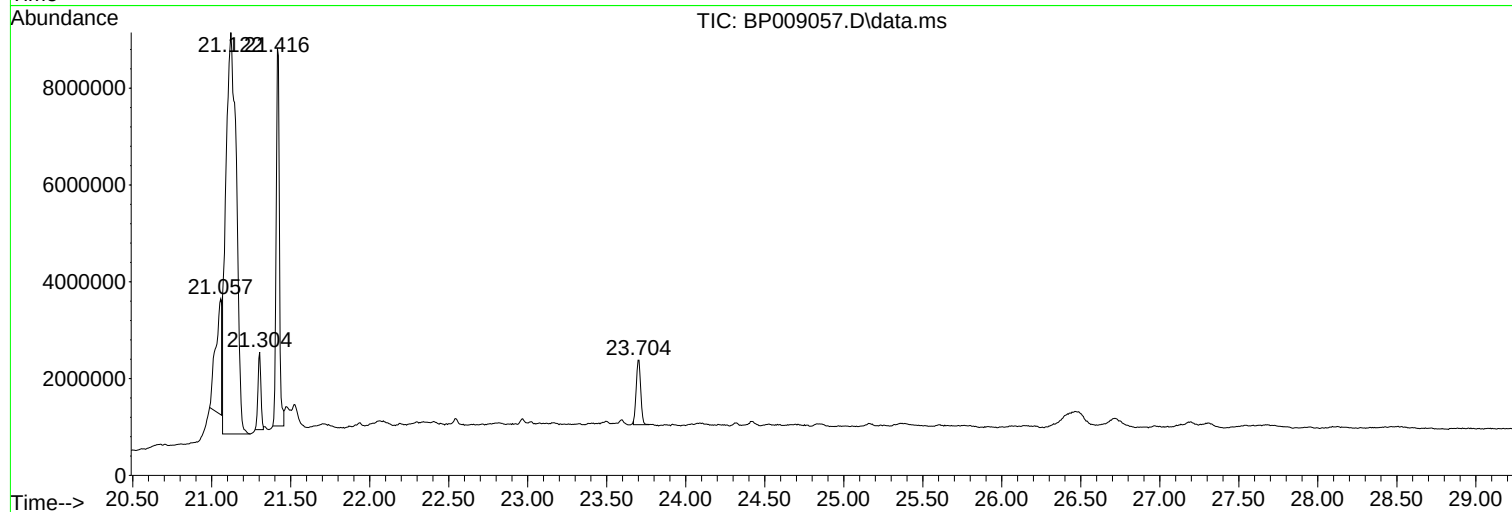
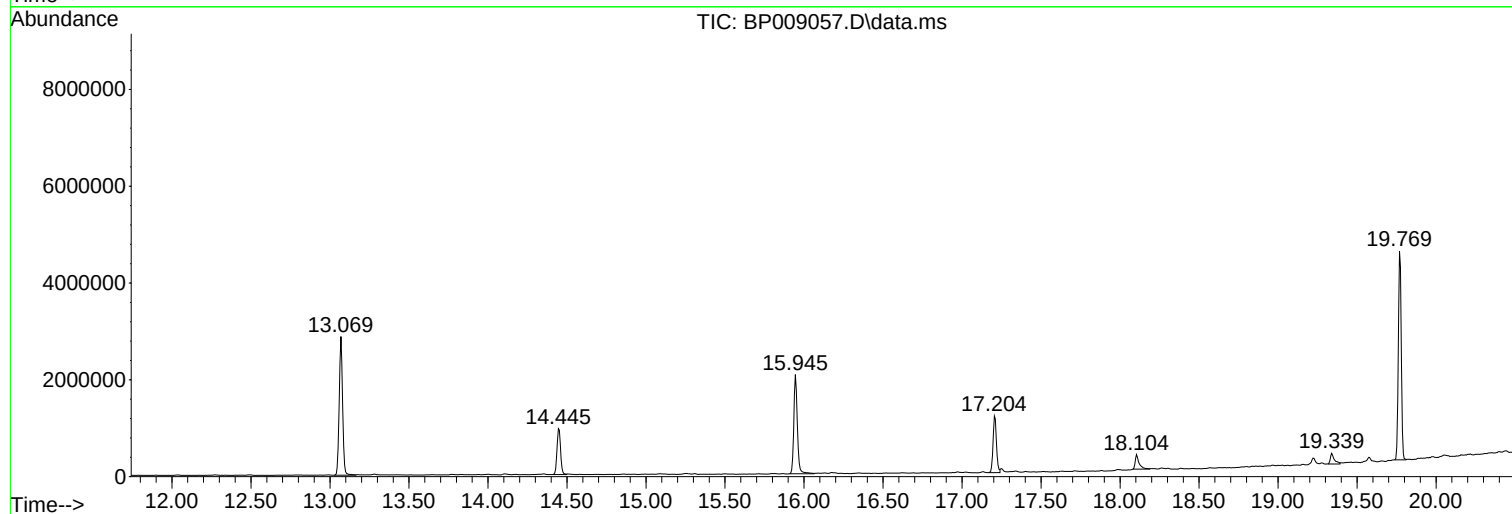
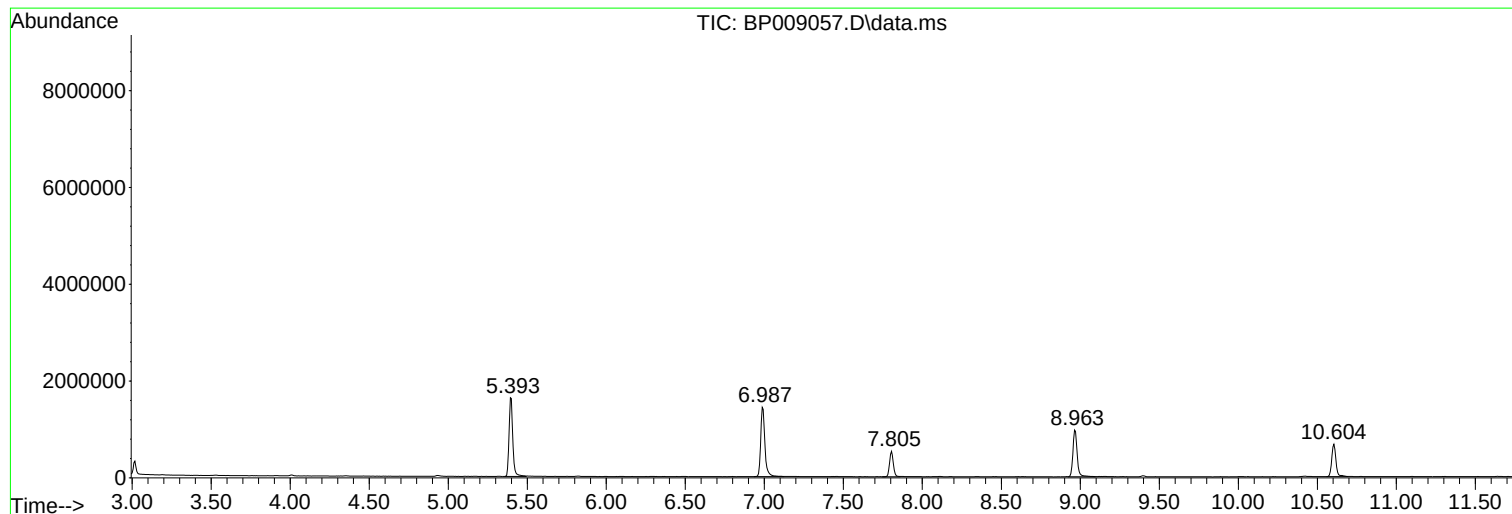
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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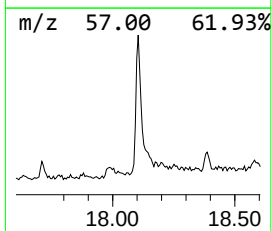
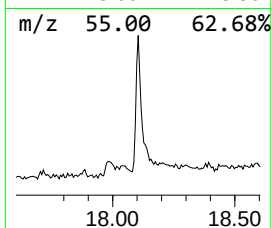
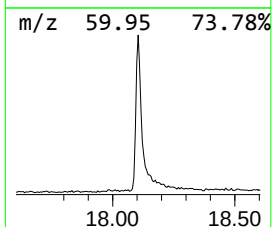
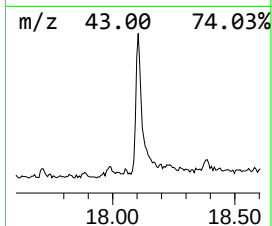
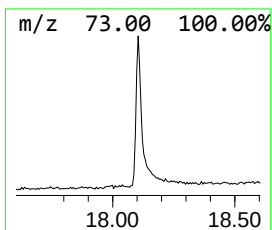
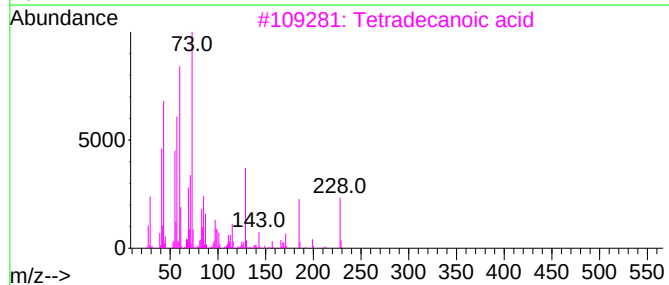
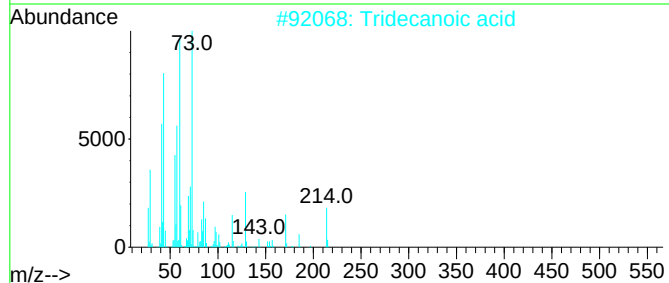
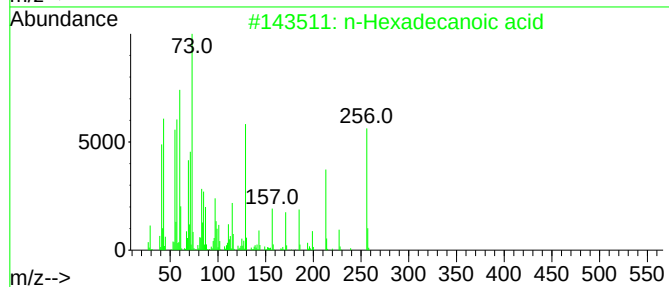
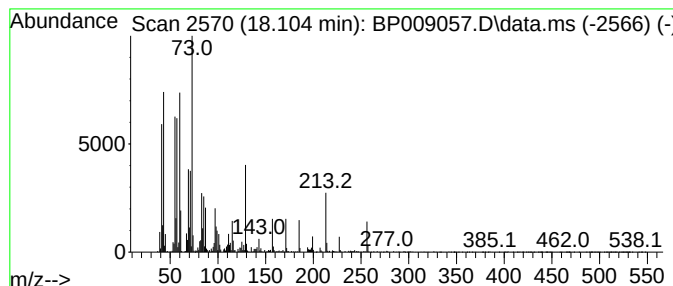
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	5.96 ng	522396	Phenanthrene-d10	17.204

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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BNA_P
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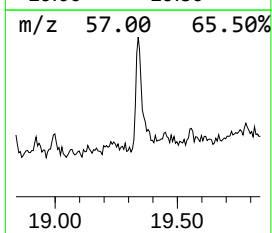
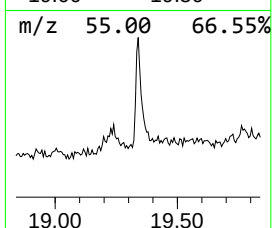
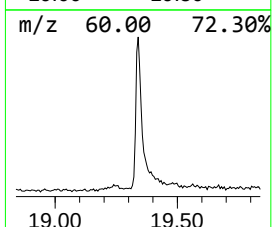
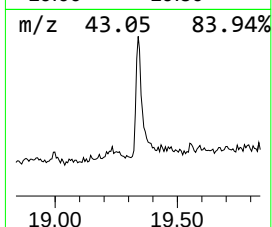
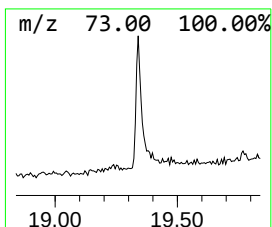
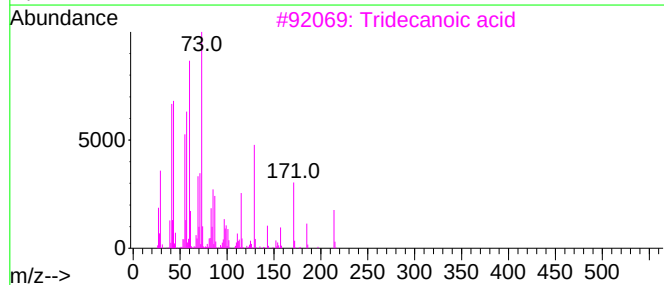
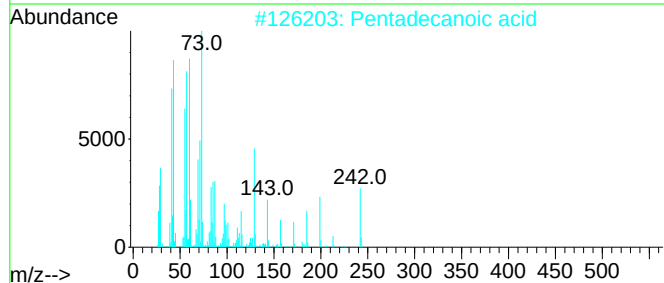
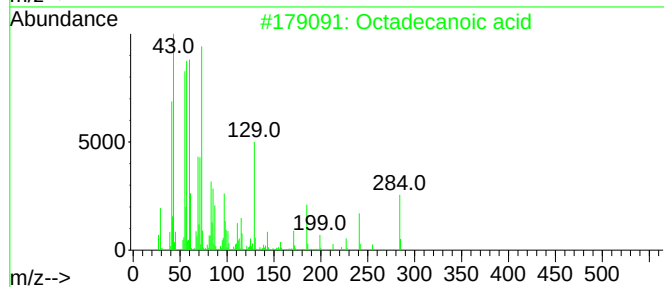
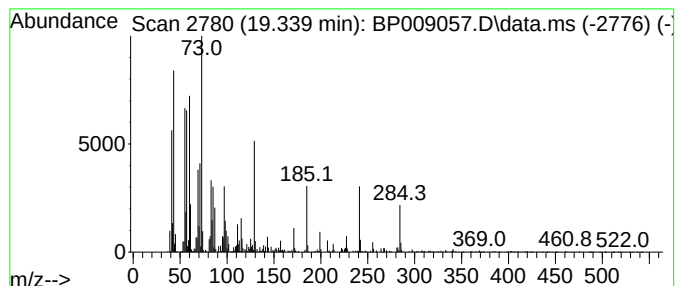
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	3.73 ng	393442	Chrysene-d12	21.304

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	70
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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Instrument :
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ClientSampleId :
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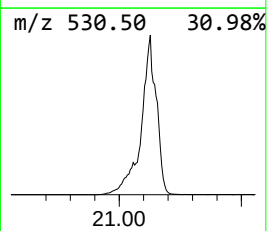
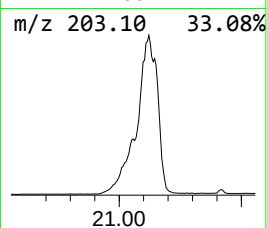
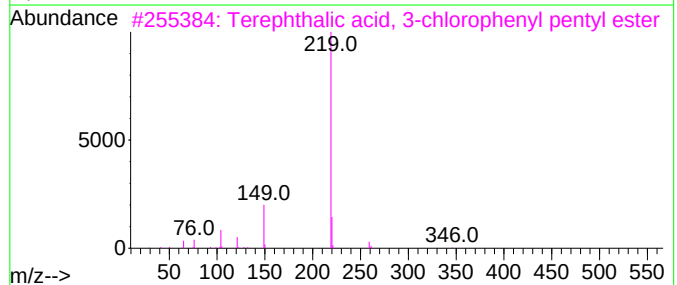
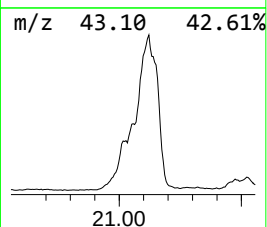
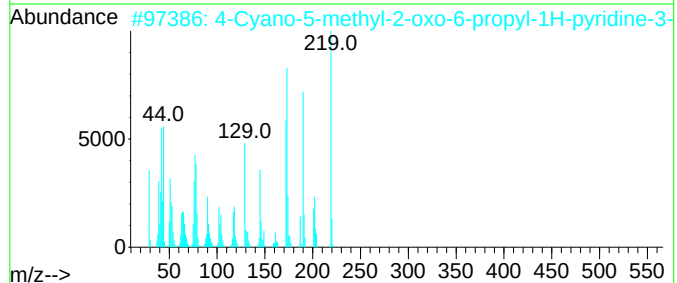
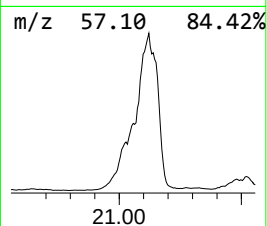
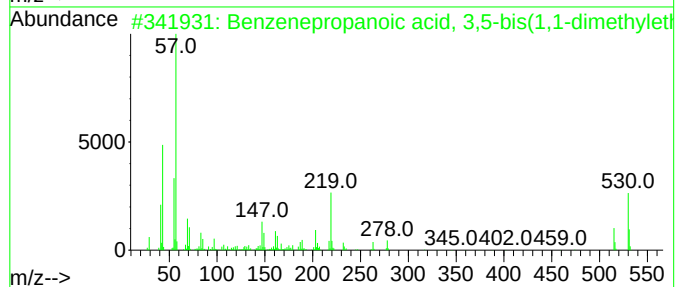
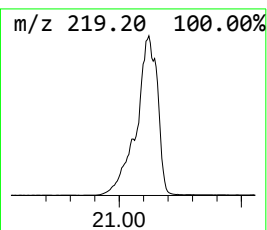
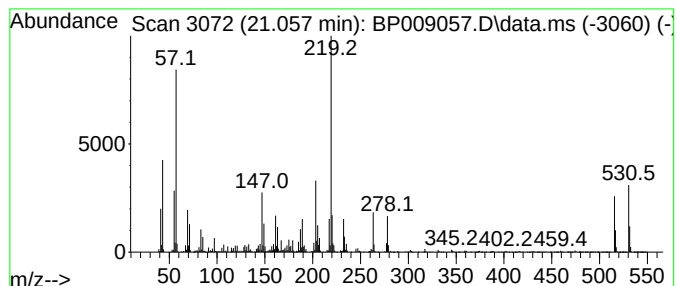
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzenepropanoic acid, 3,5-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	60.19 ng	6345390	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	97
2			4-Cyano-5-methyl-2-oxo-6-propyl-...	219	C11H13N3O2	1000459-78-4	83
3			Terephthalic acid, 3-chloropheny...	346	C19H19ClO4	1000323-64-4	38
4			4-(1H-Inden-1-ylidenemethyl)phen...	219	C16H13N	000487-61-6	38
5			Isophthalic acid, oct-3-en-2-yl ...	346	C21H30O4	1000343-89-3	35



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Instrument :
BNA_P
ClientSampleId :
KTS1-MH-01-0-15

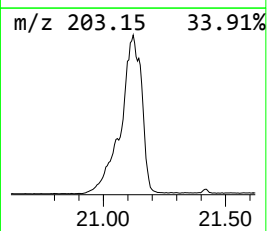
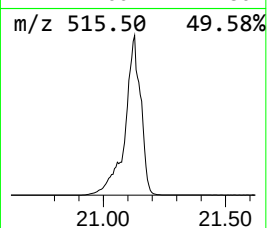
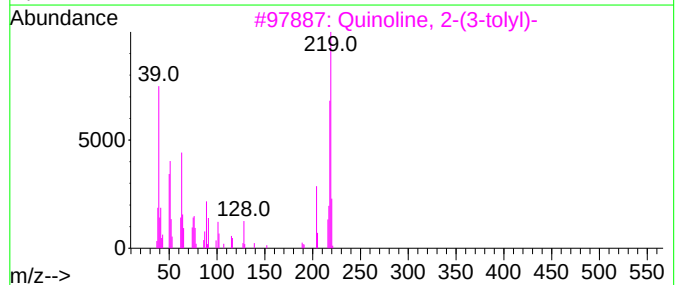
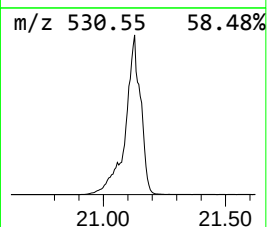
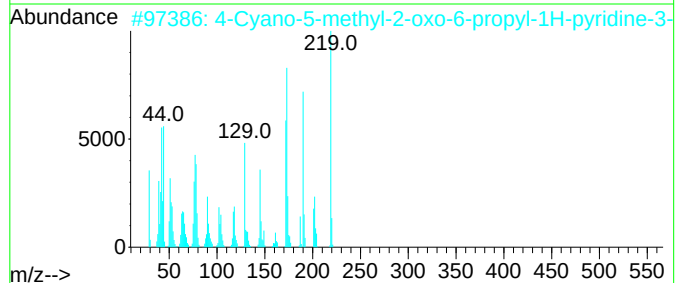
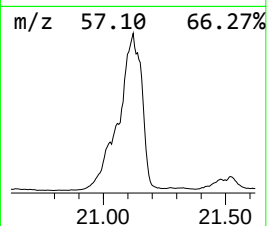
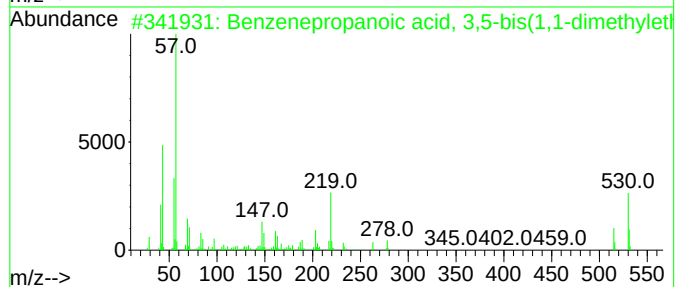
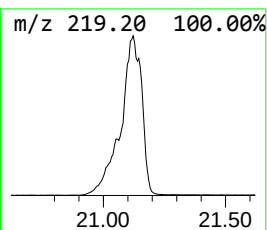
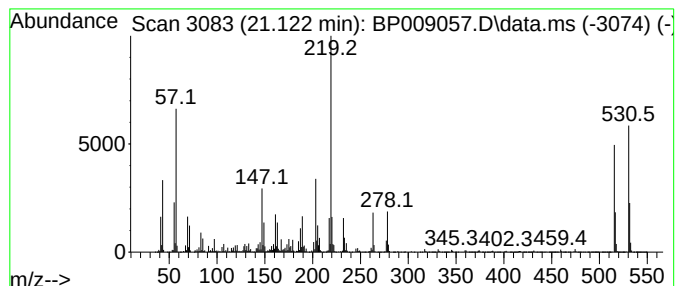
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Peak Number 4 4-Cyano-5-methyl-2-oxo-6-pr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	359.72 ng	37925000	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	92
2			4-Cyano-5-methyl-2-oxo-6-propyl-...	219	C11H13N3O2	1000459-78-4	70
3			Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	30
4			(2-Nitro-4-trifluoromethyl-pheno...	279	C9H8F3N3O4	1000294-73-1	30
5			acetamide, 2,2,2-trifluoro-N-(4-...	219	C9H8F3NO2	1010400-75-8	25



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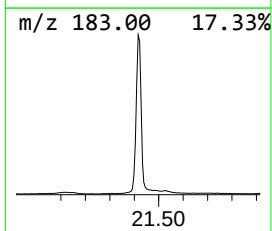
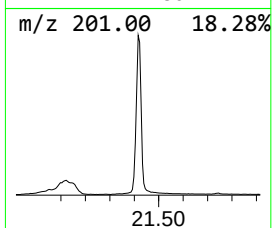
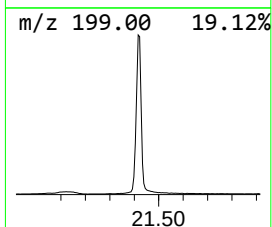
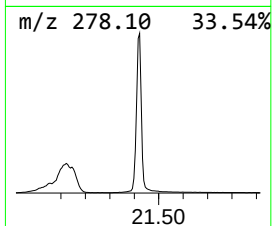
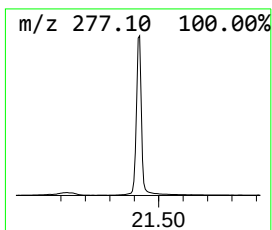
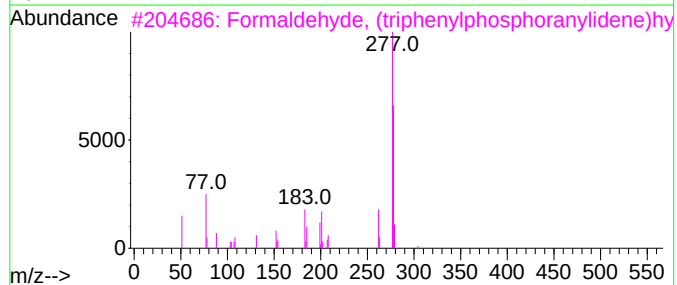
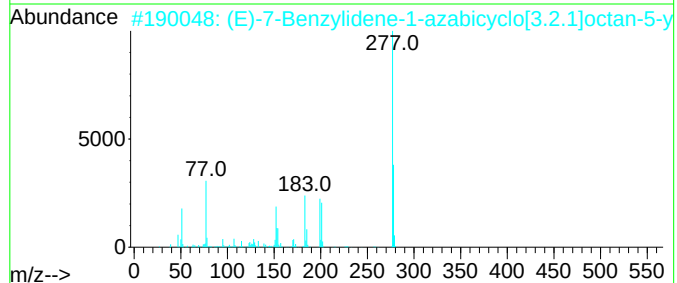
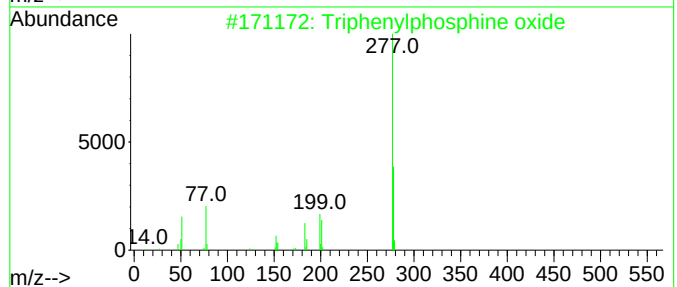
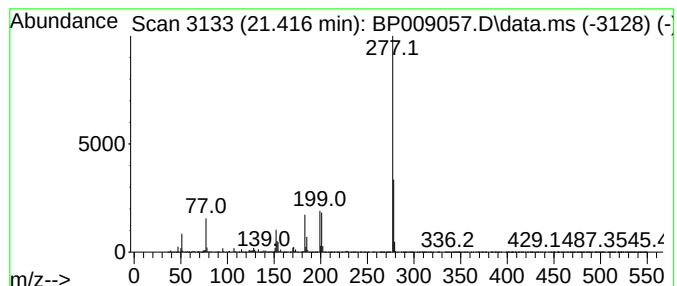
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	105.70 ng	11144200	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	47
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	9



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.104	6.0	ng	522396	4	17.204	1752400	20.0
Octadecanoic acid	19.339	3.7	ng	393442	5	21.304	2108580	20.0
Benzenepropanoi...	21.057	60.2	ng	6345390	5	21.304	2108580	20.0
4-Cyano-5-methy...	21.122	359.7	ng	37925000	5	21.304	2108580	20.0
Triphenylphosph...	21.416	105.7	ng	11144200	5	21.304	2108580	20.0