

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
 Data File : BP011674.D
 Acq On : 09 Sep 2022 21:25
 Operator : CG/JU
 Sample : N4549-15
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-59

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-BP090222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	13	rVB	1208075	1473994	3.47%	0.959%
2	3.093	13	18	31	rVV	12423558	15509328	36.54%	10.089%
3	5.052	344	351	360	rBV	289157	427699	1.01%	0.278%
4	5.516	423	430	440	rBV	3933769	5822600	13.72%	3.788%
5	7.110	694	701	716	rVB	2288314	3737186	8.80%	2.431%
6	7.957	838	845	853	rBV	1372659	2172442	5.12%	1.413%
7	9.128	1036	1044	1057	rVB	4463744	7506872	17.69%	4.883%
8	10.769	1316	1323	1330	rBV	1754132	3046586	7.18%	1.982%
9	12.098	1543	1549	1555	rBV	269101	442328	1.04%	0.288%
10	13.228	1731	1741	1753	rVB	11212179	16819310	39.63%	10.941%
11	14.598	1963	1974	1981	rBV	2536227	3894491	9.18%	2.533%
12	16.086	2221	2227	2236	rBV	7884452	11498896	27.09%	7.480%
13	17.351	2436	2442	2448	rBV	2925905	4167298	9.82%	2.711%
14	18.233	2588	2592	2602	rBV	869635	1400718	3.30%	0.911%
15	18.404	2616	2621	2627	rVB2	239058	438880	1.03%	0.286%
16	19.357	2778	2783	2788	rVB	745333	954915	2.25%	0.621%
17	19.463	2797	2801	2812	rBV	503793	845929	1.99%	0.550%
18	19.710	2838	2843	2851	rVB	892837	1428080	3.36%	0.929%
19	19.904	2870	2876	2883	rVB	16200960	19959955	47.02%	12.984%
20	21.145	3083	3087	3093	rBV3	342269	471522	1.11%	0.307%
21	21.433	3131	3136	3141	rBV	3498411	4502384	10.61%	2.929%
22	21.563	3151	3158	3183	rBV	24010210	42445937	100.00%	27.612%
23	23.898	3549	3555	3565	rVB2	2303814	4755183	11.20%	3.093%

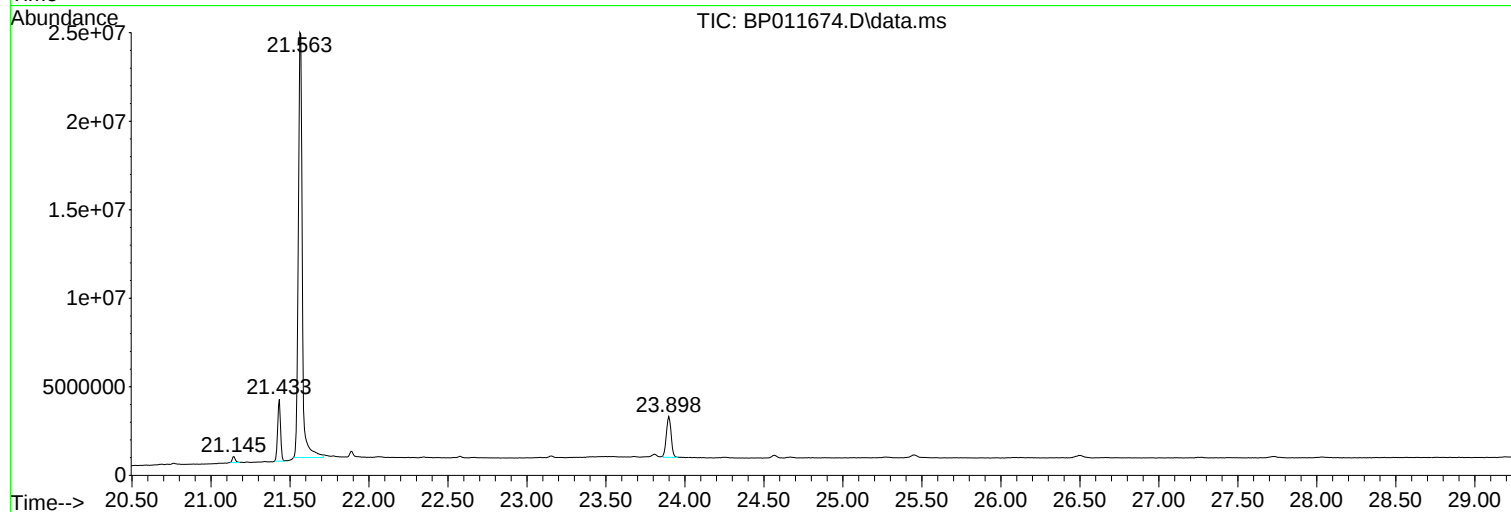
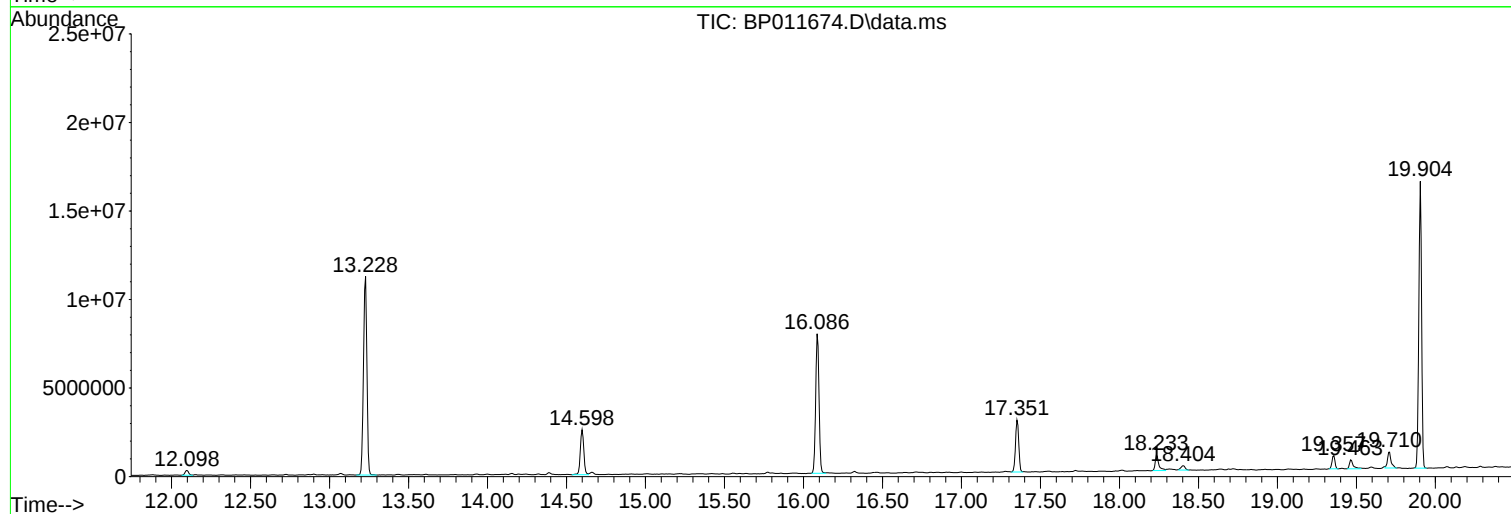
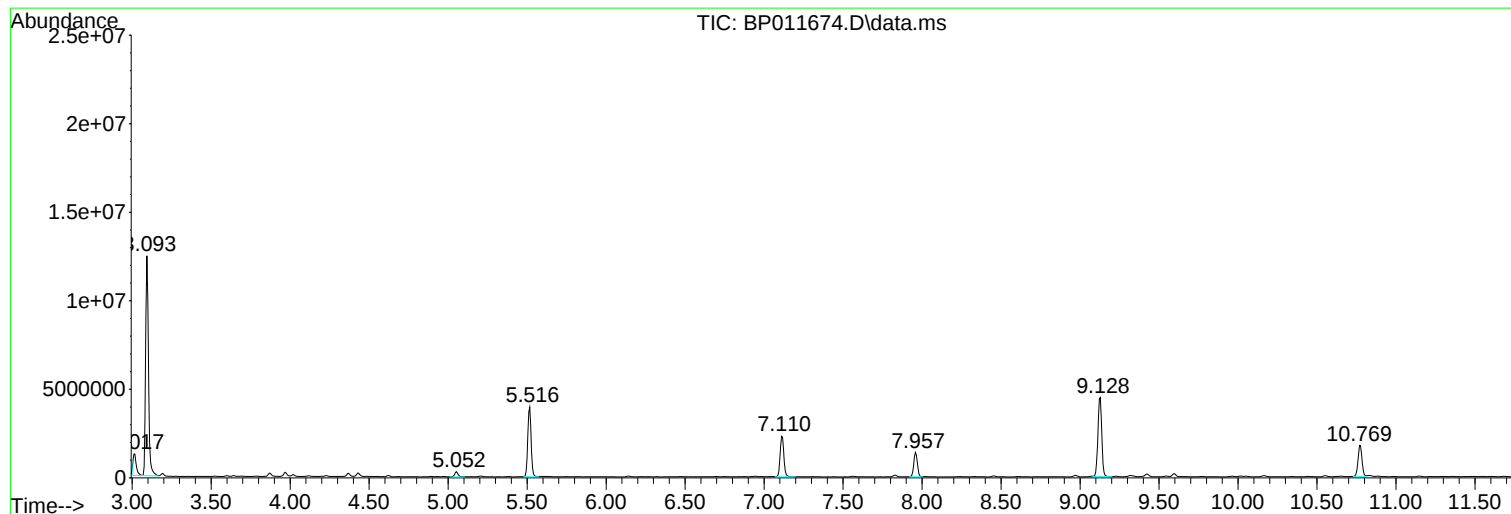
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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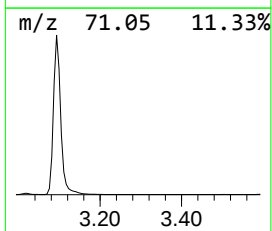
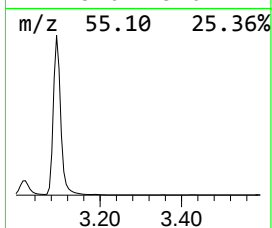
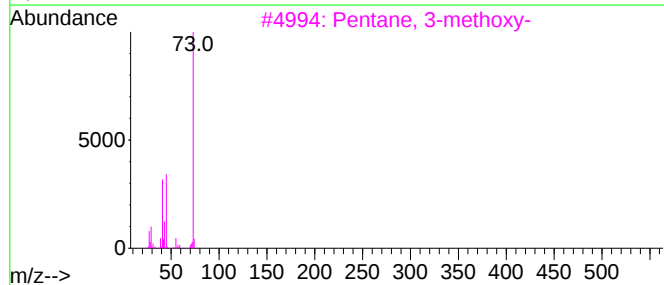
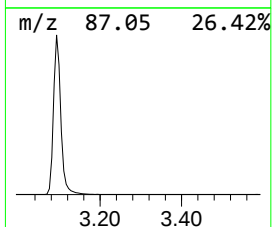
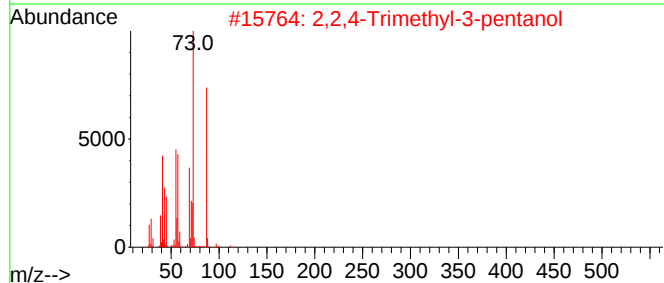
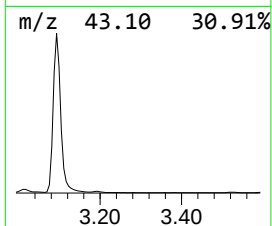
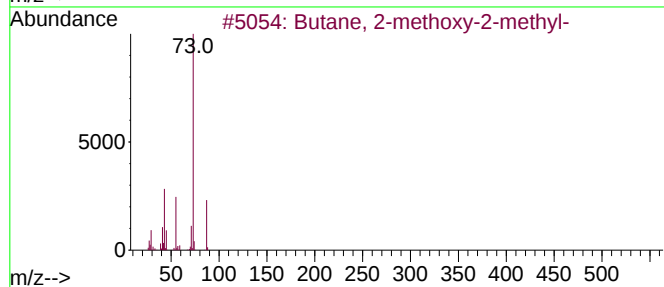
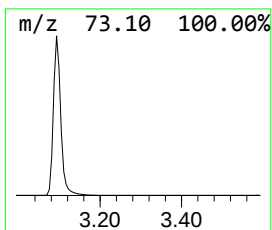
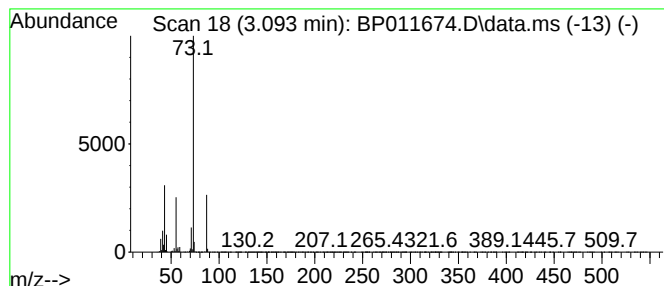
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	142.78 ng	15509300	1,4-Dichlorobenzene-d4	7.957

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	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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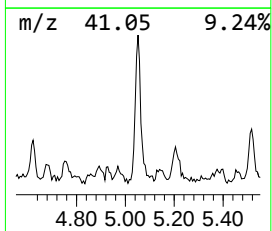
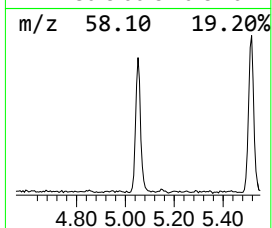
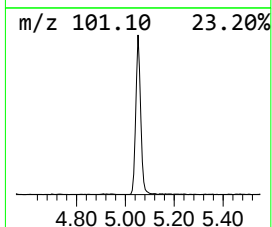
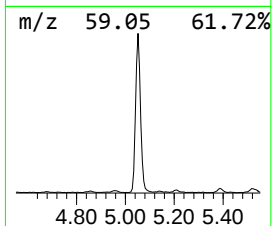
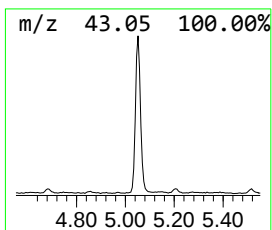
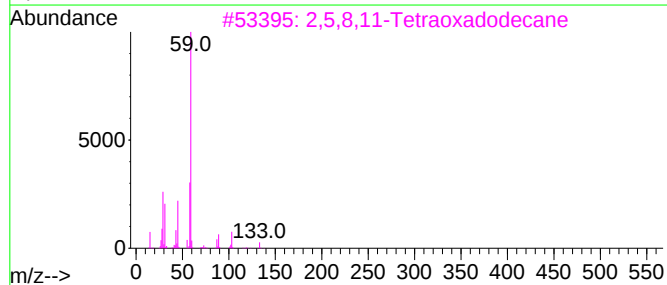
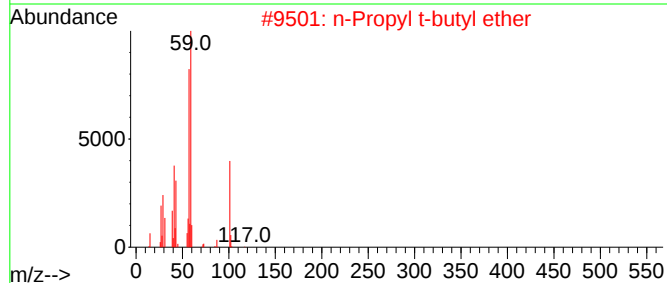
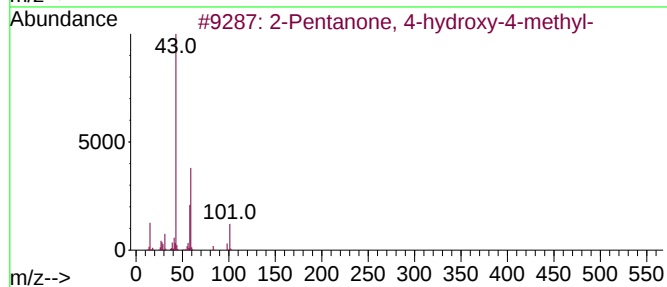
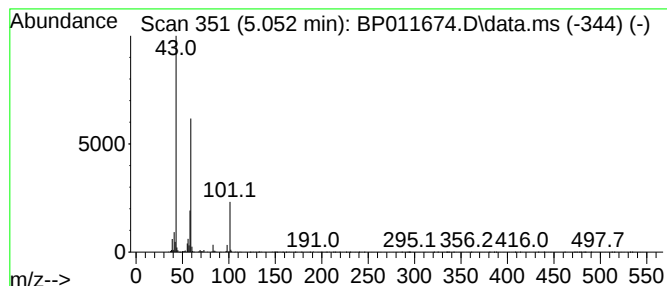
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	3.94 ng	427699	1,4-Dichlorobenzene-d4	7.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25
4		Tetraglyme	222	C10H22O5	000143-24-8	25
5		1,2-Butanediol	90	C4H10O2	000584-03-2	17



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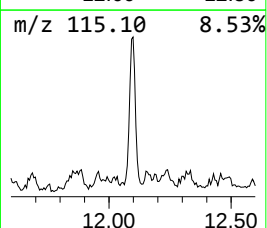
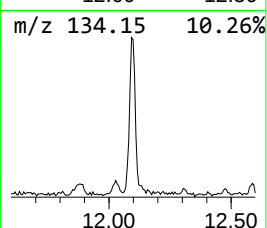
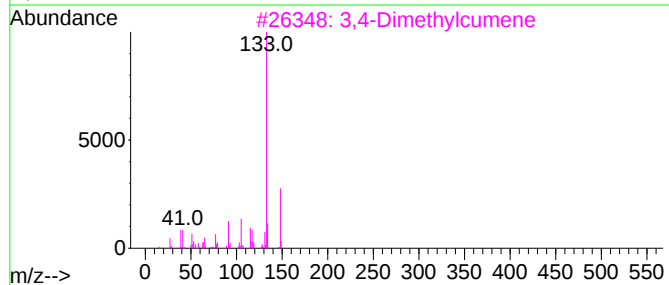
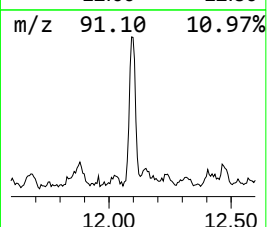
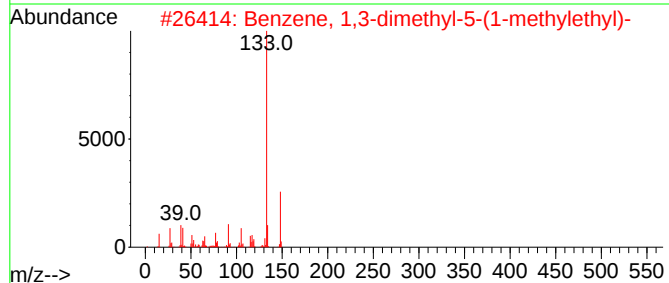
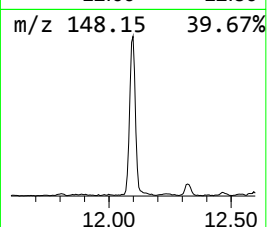
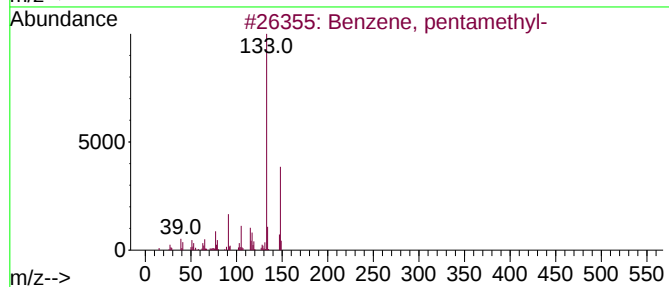
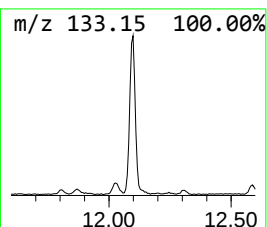
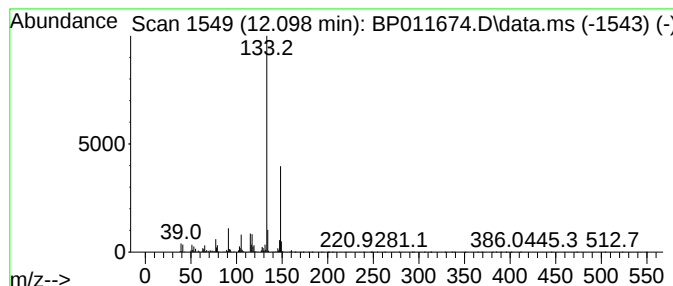
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzene, pentamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	2.90 ng	442328	Naphthalene-d8	10.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, pentamethyl-	148	C11H16	000700-12-9	95
2			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	91
3			3,4-Dimethylcumene	148	C11H16	1000370-34-1	90
4			1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	90
5			Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	90



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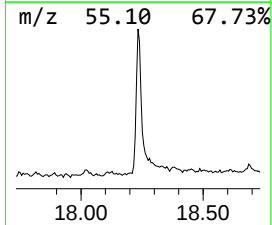
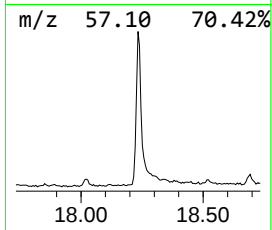
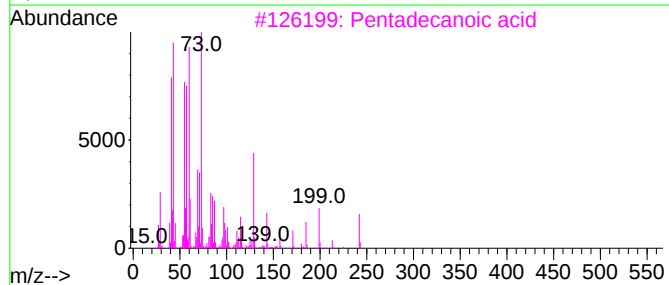
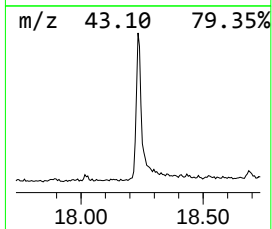
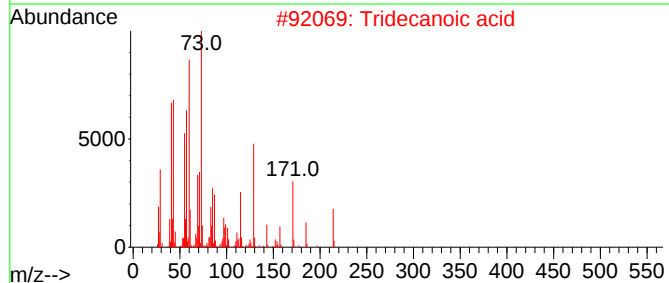
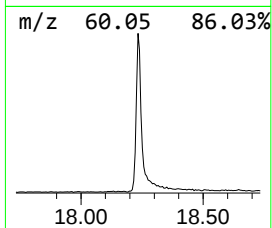
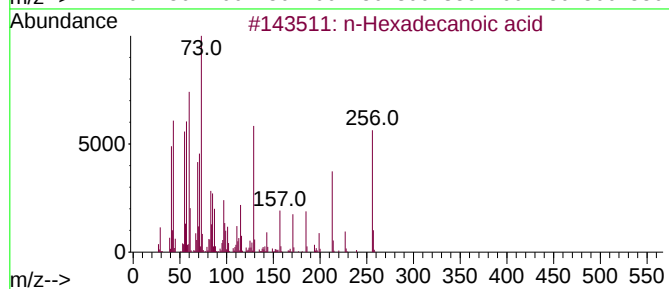
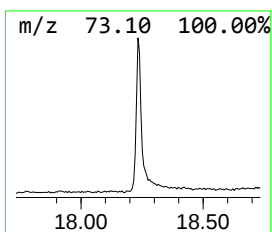
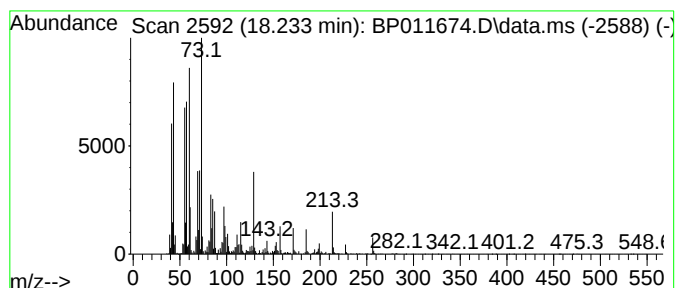
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	6.72 ng	1400720	Phenanthrene-d10	17.351

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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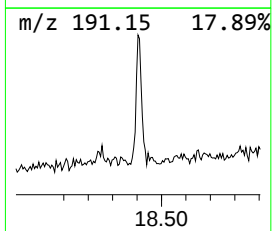
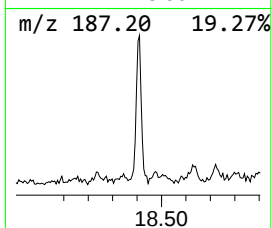
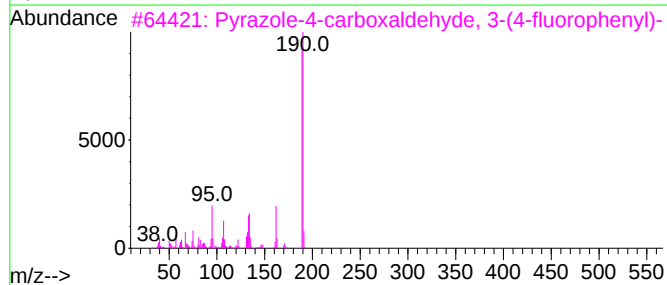
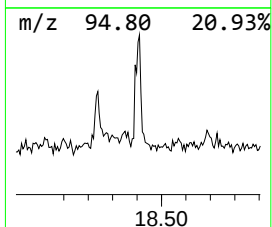
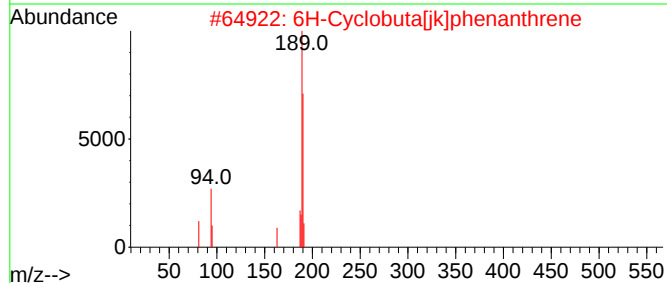
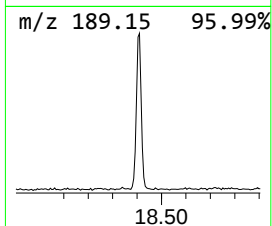
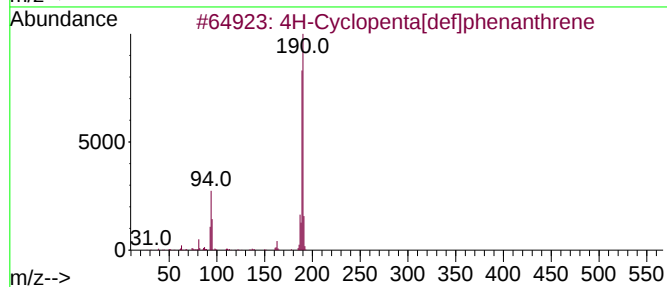
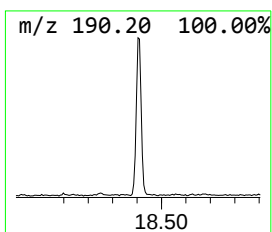
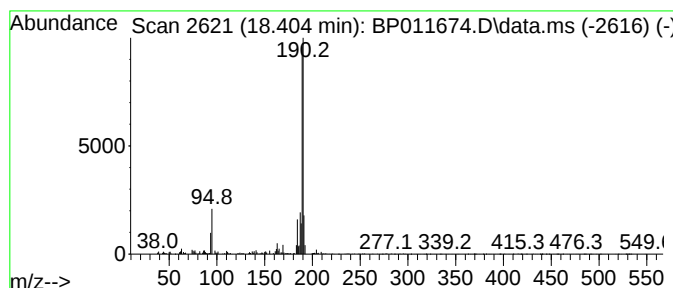
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.404	2.11 ng	438880	Phenanthrene-d10	17.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	59
4	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	53
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42



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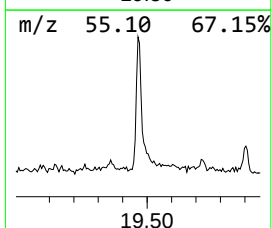
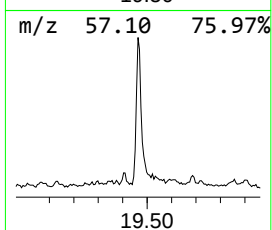
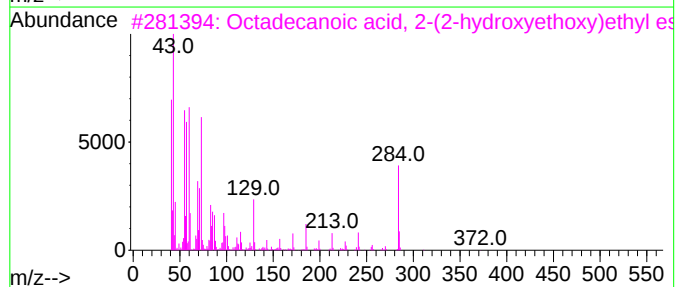
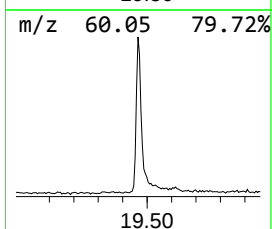
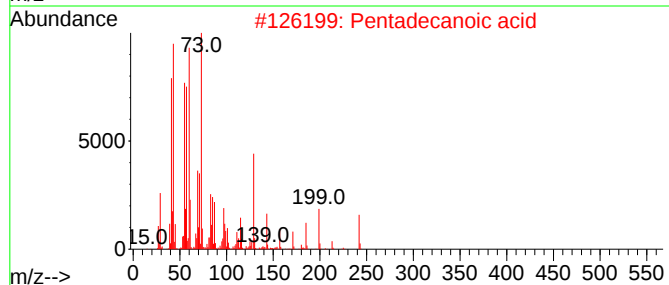
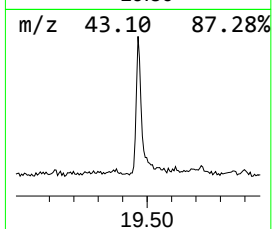
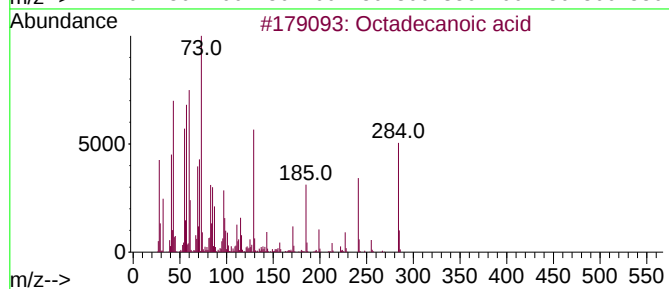
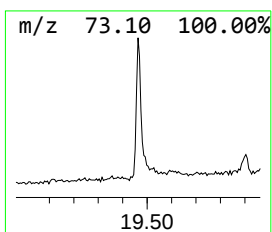
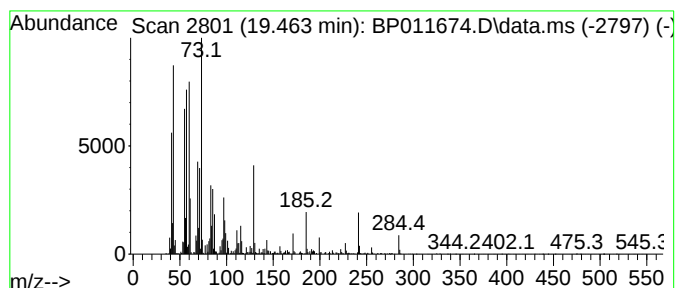
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	3.76 ng	845929	Chrysene-d12	21.433

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011674.D
Acq On : 09 Sep 2022 21:25
Operator : CG/JU
Sample : N4549-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-59

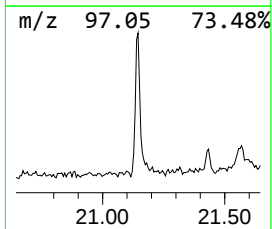
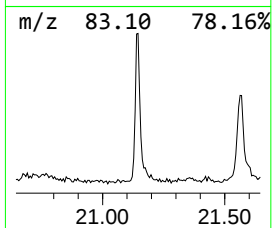
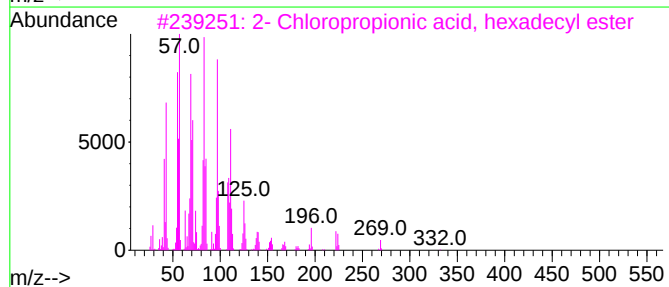
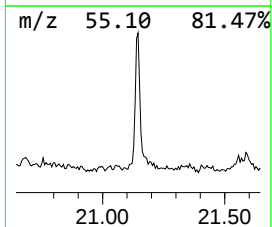
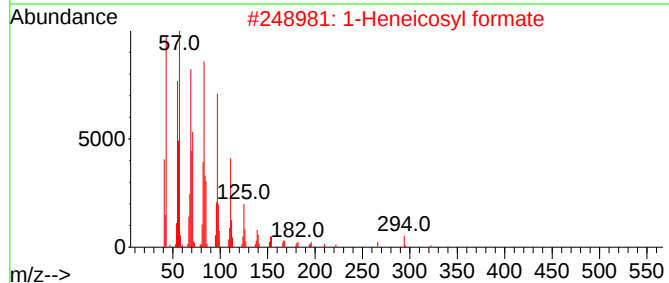
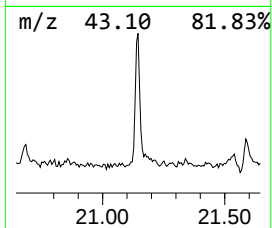
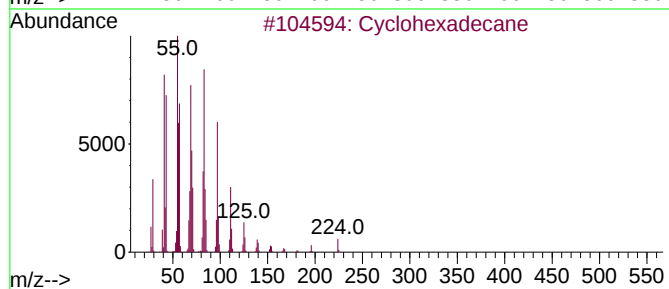
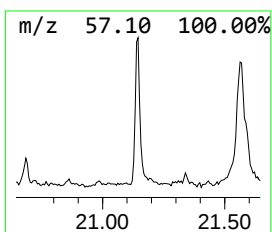
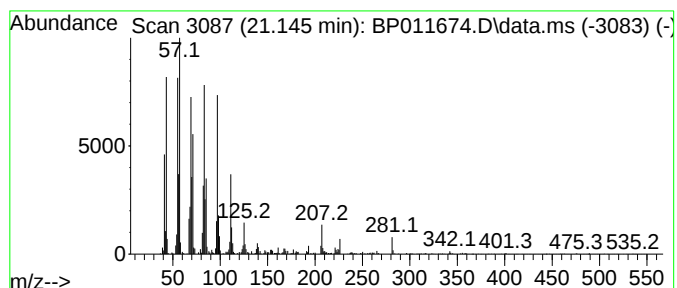
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	2.09 ng	471522	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011674.D
Acq On : 09 Sep 2022 21:25
Operator : CG/JU
Sample : N4549-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-59

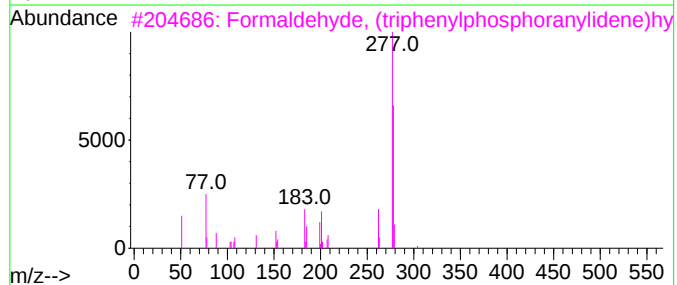
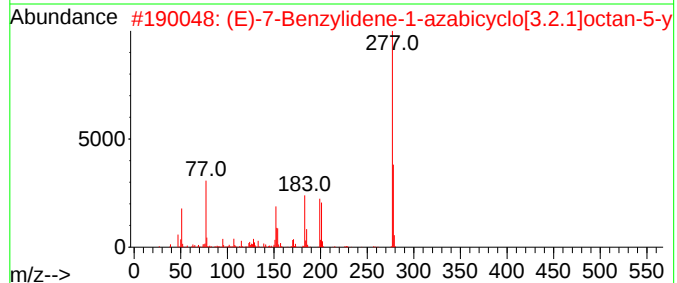
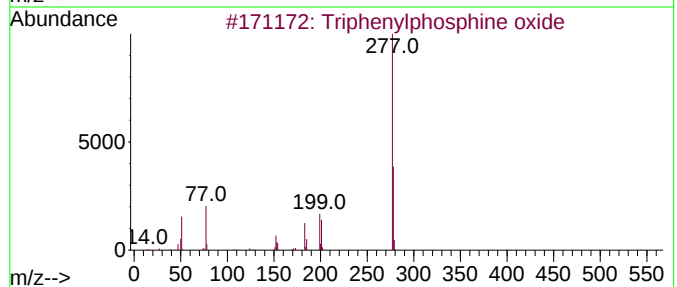
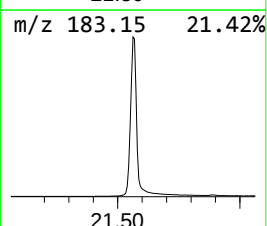
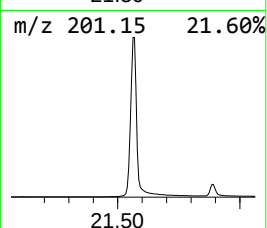
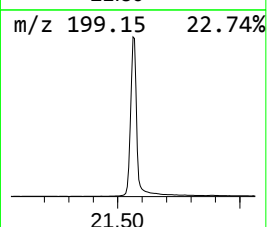
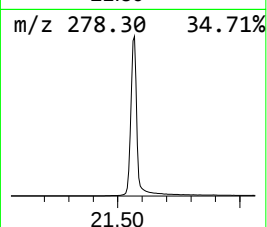
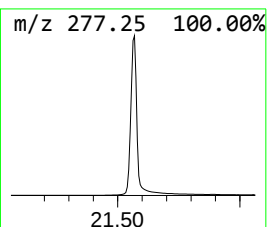
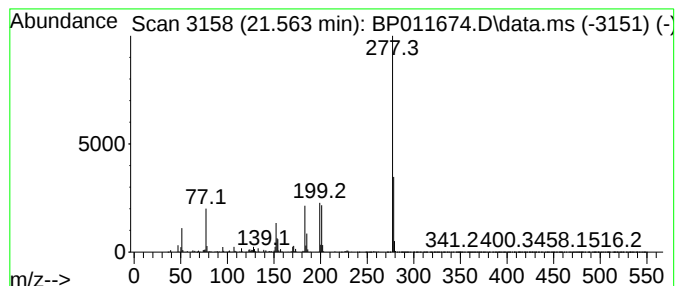
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	188.55 ng	42445900	Chrysene-d12	21.433

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	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011674.D
Acq On : 09 Sep 2022 21:25
Operator : CG/JU
Sample : N4549-15
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-59

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.093	142.8	ng	15509300	1	7.957	2172440	20.0
2-Pentanone, 4-...	5.052	3.9	ng	427699	1	7.957	2172440	20.0
Benzene, pentam...	12.098	2.9	ng	442328	2	10.769	3046590	20.0
n-Hexadecanoic ...	18.233	6.7	ng	1400720	4	17.351	4167300	20.0
4H-Cyclopenta[d...	18.404	2.1	ng	438880	4	17.351	4167300	20.0
Octadecanoic acid	19.463	3.8	ng	845929	5	21.433	4502380	20.0
Cyclohexadecane	21.145	2.1	ng	471522	5	21.433	4502380	20.0
Triphenylphosph...	21.563	188.6	ng	42445900	5	21.433	4502380	20.0