

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021022\
 Data File : BP009101.D
 Acq On : 10 Feb 2022 16:08
 Operator : CG/JU
 Sample : N1435-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RO-369

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: BP009101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	3	4	20	rVB	267023	338813	2.85%	0.375%
2	3.558	92	97	115	rBV	733210	1069376	9.00%	1.183%
3	5.399	404	410	433	rBV	2714740	4598152	38.69%	5.086%
4	6.999	674	682	704	rBV	2569205	4668572	39.28%	5.163%
5	7.799	810	818	827	rBV	670042	1158350	9.75%	1.281%
6	8.963	1008	1016	1041	rBV	1644968	3089476	26.00%	3.417%
7	10.599	1285	1294	1309	rBV	871437	1647342	13.86%	1.822%
8	13.063	1706	1713	1728	rBV	5079586	8200612	69.00%	9.070%
9	14.169	1896	1901	1909	rVB	101004	164482	1.38%	0.182%
10	14.445	1937	1948	1954	rBV	1507966	2393071	20.14%	2.647%
11	14.504	1954	1958	1967	rVB	104956	197464	1.66%	0.218%
12	15.498	2122	2127	2139	rVB2	95772	195302	1.64%	0.216%
13	15.945	2193	2203	2222	rBV	4181216	6584283	55.40%	7.282%
14	17.204	2411	2417	2421	rVV	1884815	2784437	23.43%	3.080%
15	17.245	2421	2424	2431	rVV	912342	1272146	10.70%	1.407%
16	17.339	2435	2440	2445	rVB	213471	324707	2.73%	0.359%
17	17.616	2481	2487	2494	rBV	94500	199704	1.68%	0.221%
18	18.075	2561	2565	2567	rBV	242280	326581	2.75%	0.361%
19	18.104	2567	2570	2582	rVV2	483742	1076069	9.05%	1.190%
20	18.198	2583	2586	2591	rVV	90407	133145	1.12%	0.147%
21	18.263	2591	2597	2600	rVV2	330674	590758	4.97%	0.653%
22	18.298	2600	2603	2608	rVB	189222	270384	2.28%	0.299%
23	18.557	2643	2647	2651	rBV	132514	197273	1.66%	0.218%
24	18.845	2691	2696	2700	rBV3	145412	254188	2.14%	0.281%
25	18.927	2705	2710	2720	rBV	6157605	9488264	79.84%	10.494%
26	19.216	2754	2759	2766	rBV	1572669	2276356	19.15%	2.518%
27	19.333	2776	2779	2783	rBV	203727	232552	1.96%	0.257%
28	19.451	2797	2799	2803	rVB2	133786	147269	1.24%	0.163%
29	19.569	2810	2819	2828	rBV	1483266	2692202	22.65%	2.978%
30	19.645	2829	2832	2837	rVB	143386	209647	1.76%	0.232%
31	19.769	2847	2853	2858	rBV	8270794	10134551	85.28%	11.209%
32	20.151	2915	2918	2923	rBV	221088	269546	2.27%	0.298%
33	20.216	2925	2929	2932	rVV2	180760	259301	2.18%	0.287%
34	20.351	2949	2952	2956	rBV2	191447	274888	2.31%	0.304%
35	21.010	3061	3064	3072	rVB4	491958	854468	7.19%	0.945%
36	21.298	3107	3113	3117	rBV2	2501796	4178855	35.16%	4.622%

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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

37	21.339	3117	3120	3125	rVV	784232	1008740	8.49%	1.116%
38	21.416	3128	3133	3148	rVV	8310582	11884446	100.00%	13.144%
39	22.968	3393	3397	3402	rBV	516545	1047556	8.81%	1.159%
40	23.592	3500	3503	3513	rVB	584629	1051549	8.85%	1.163%

41	23.698	3516	3521	3528	rVB2	1340313	2670692	22.47%	2.954%
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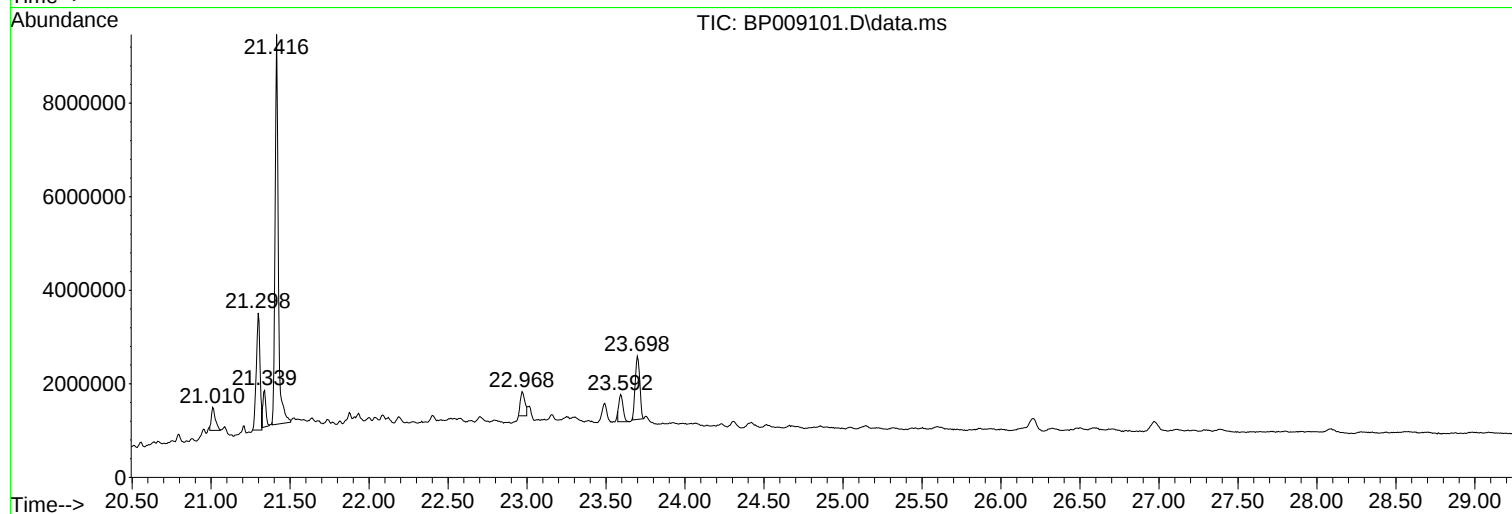
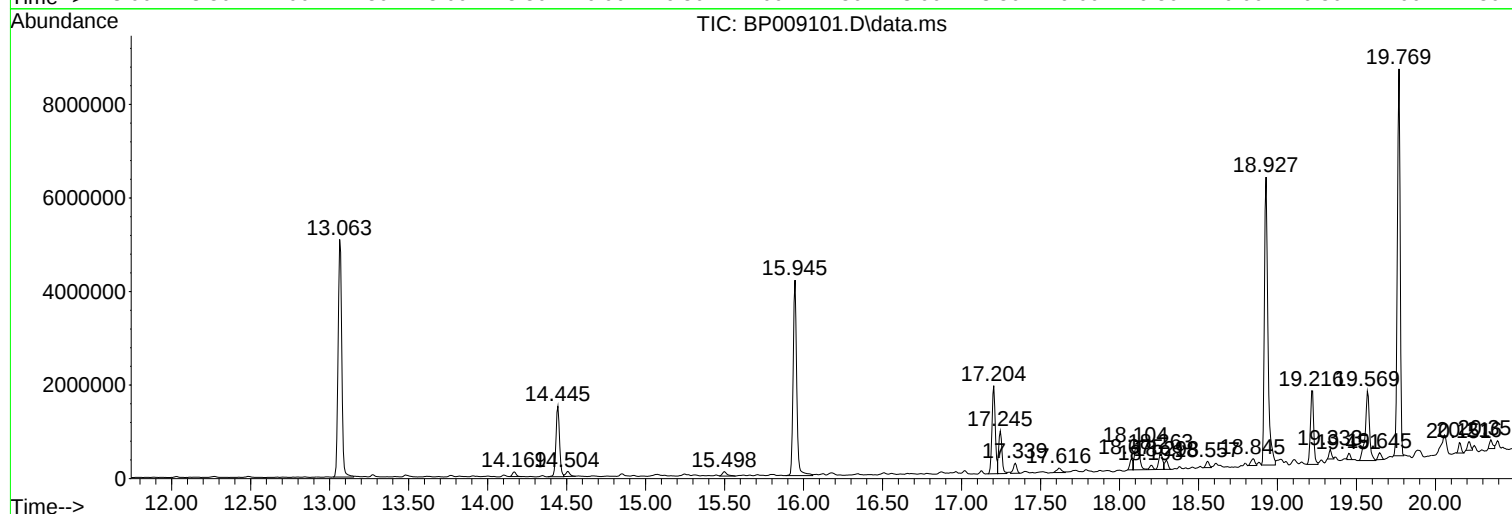
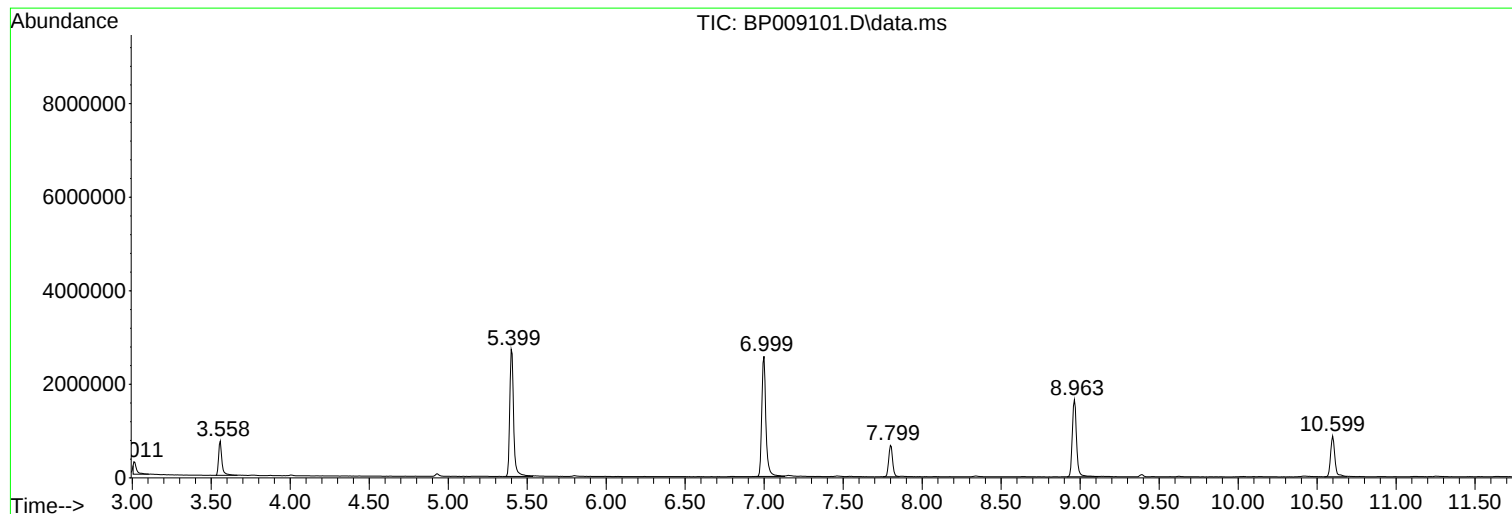
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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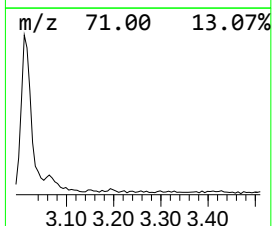
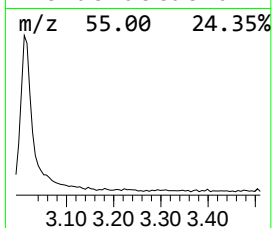
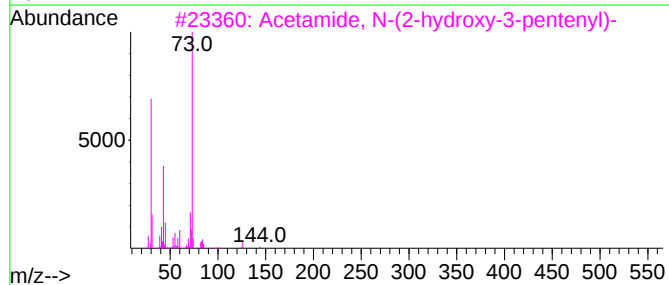
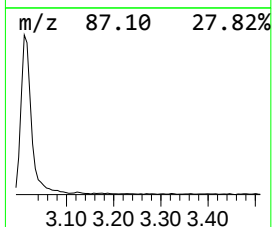
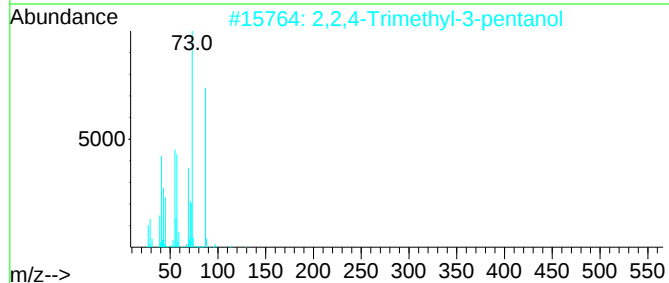
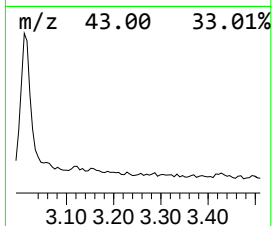
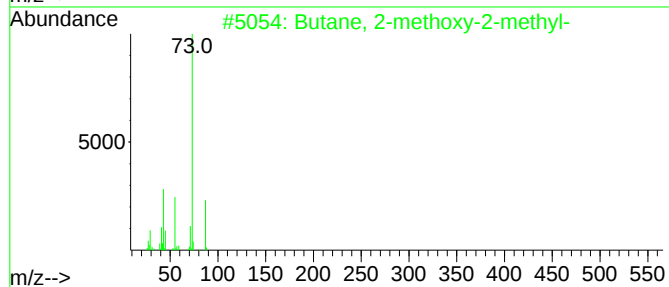
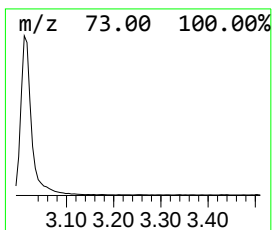
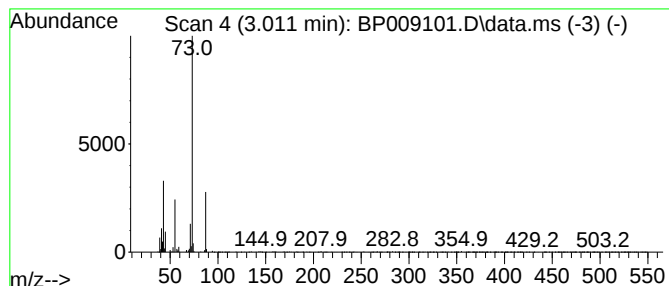
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.011	5.85 ng	338813	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	25
4			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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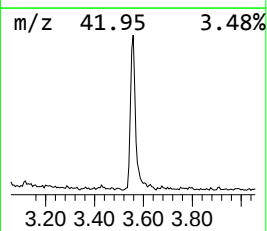
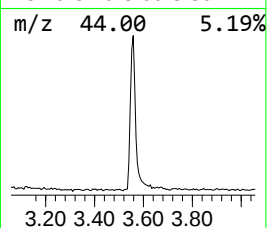
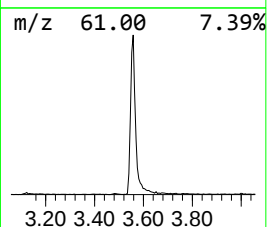
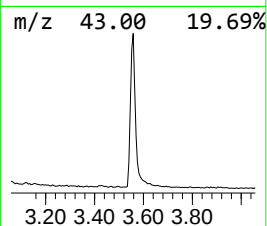
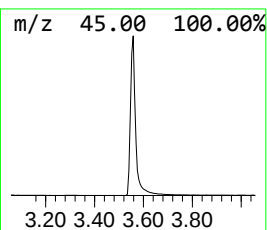
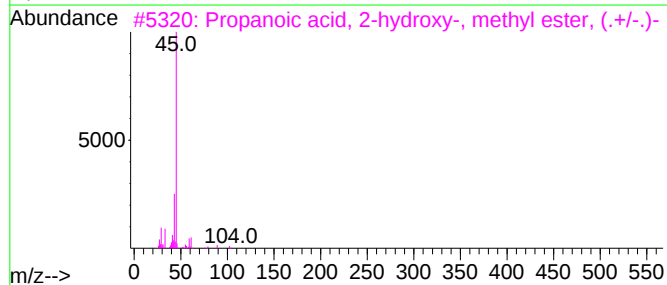
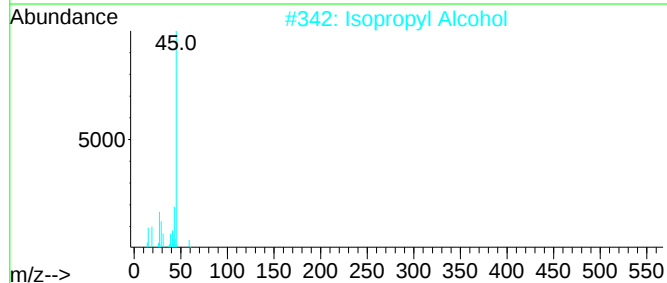
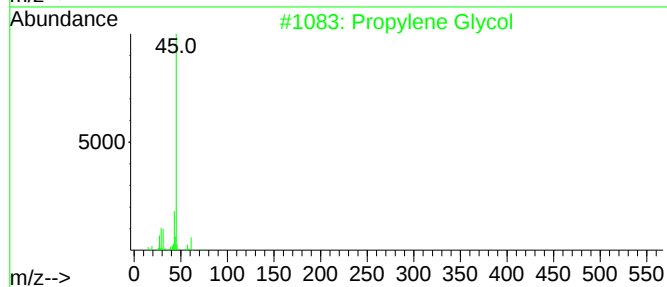
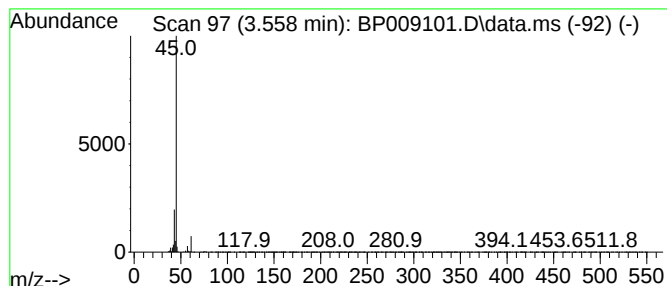
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	18.46 ng	1069380	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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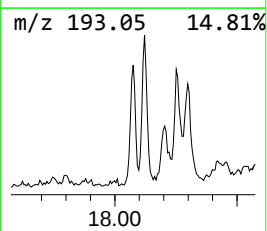
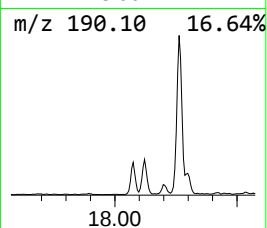
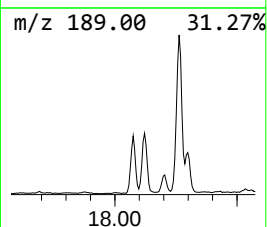
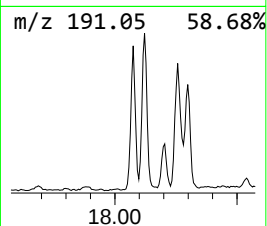
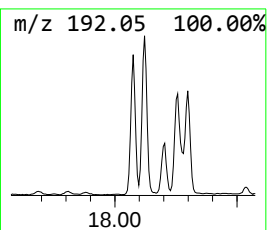
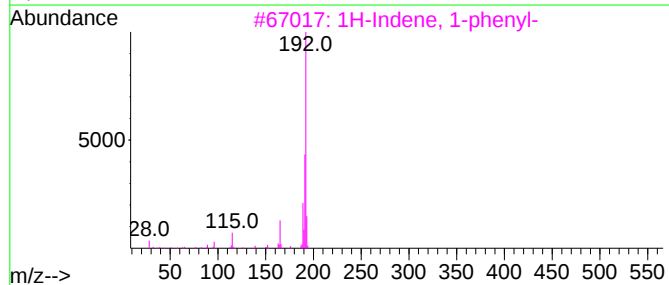
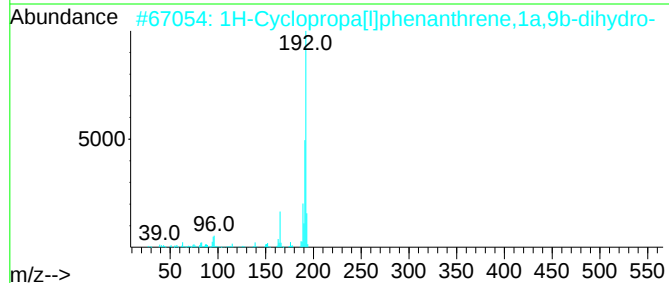
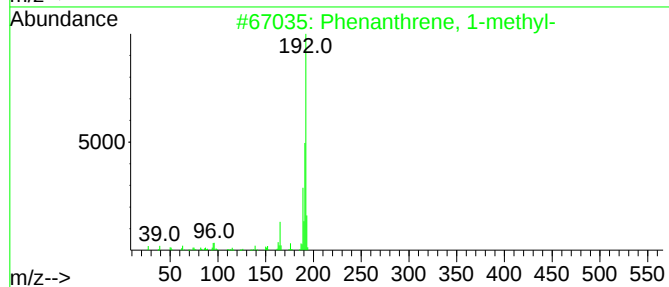
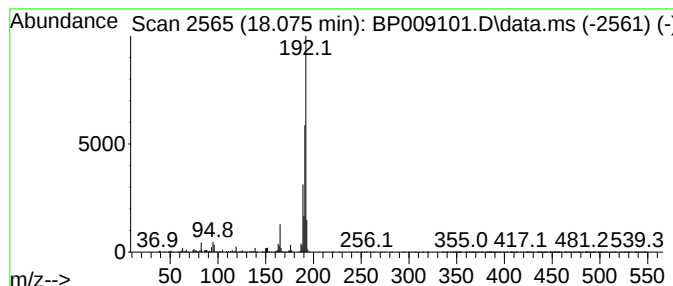
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.075	2.35 ng	326581	Phenanthrene-d10	17.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	94
3		1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	94
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	93



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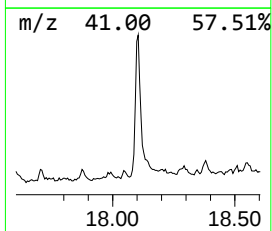
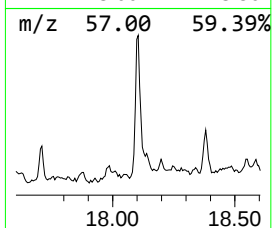
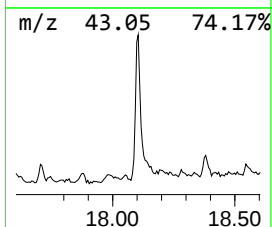
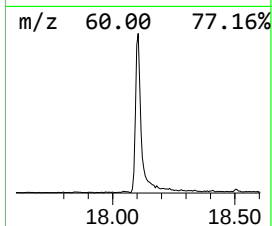
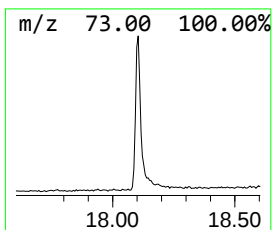
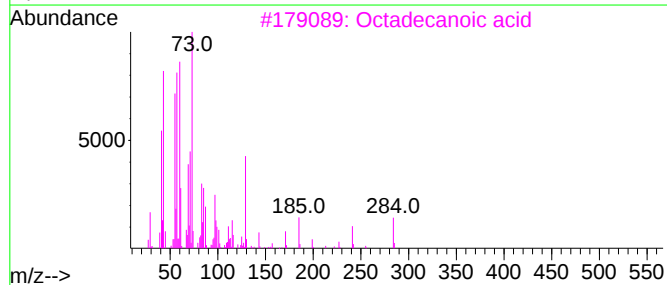
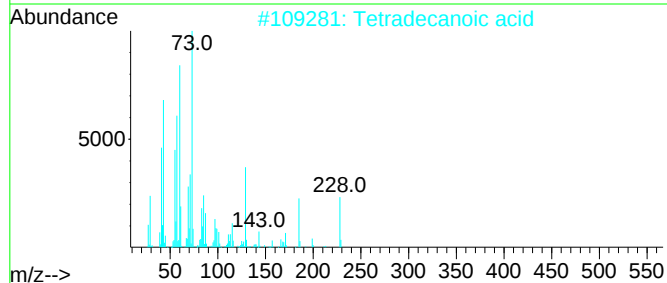
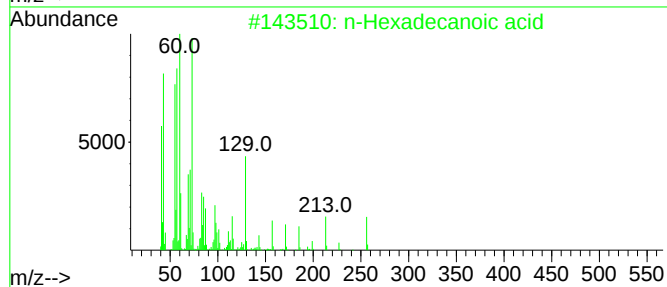
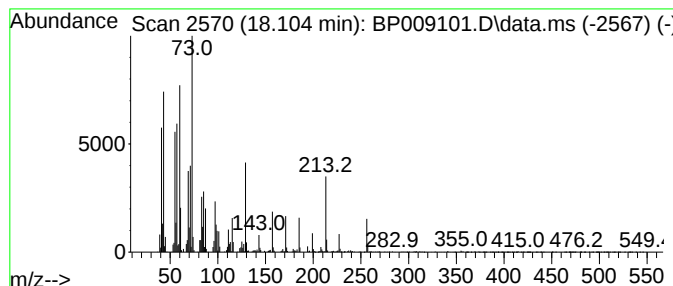
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	7.73 ng	1076070	Phenanthrene-d10	17.204

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	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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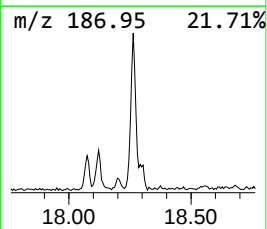
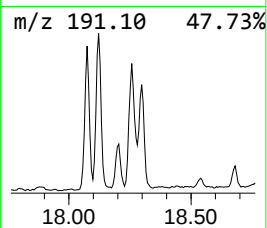
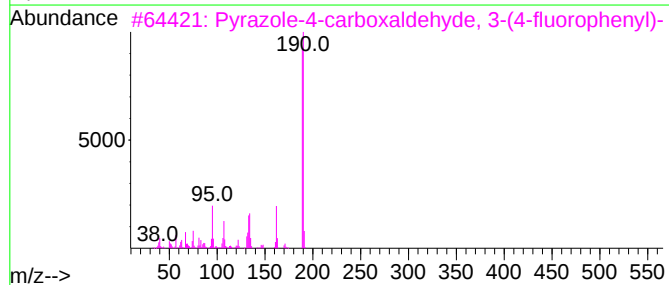
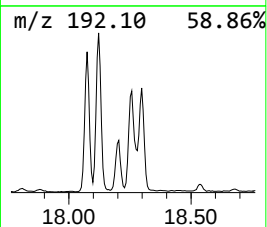
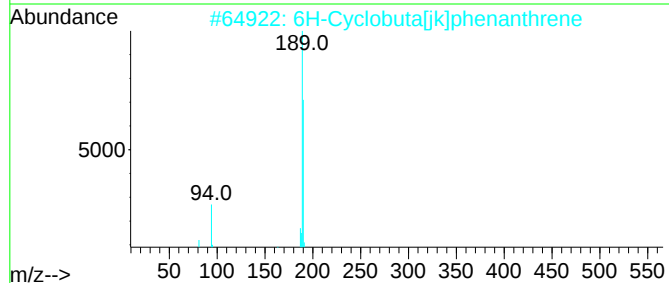
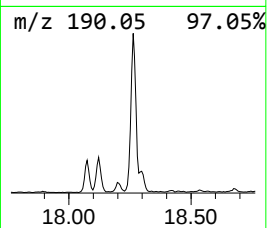
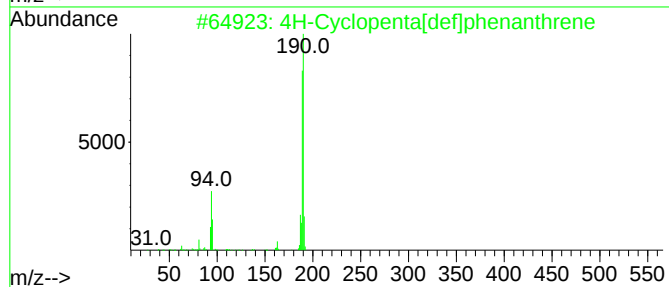
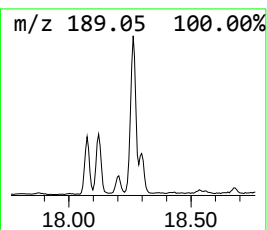
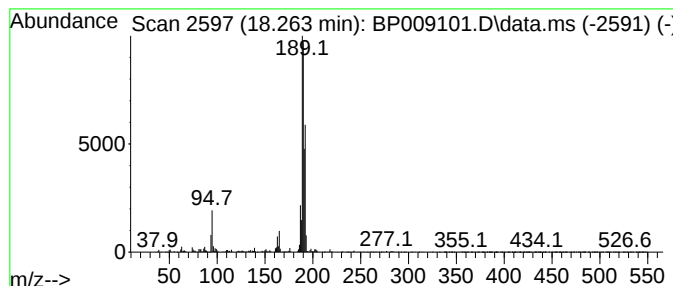
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.263	4.24 ng	590758	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	86
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
4			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	43
5			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021022\
Data File : BP009101.D
Acq On : 10 Feb 2022 16:08
Operator : CG/JU
Sample : N1435-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

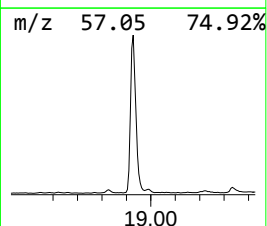
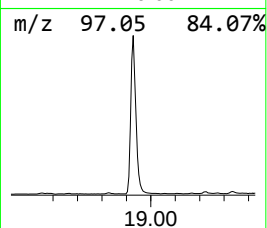
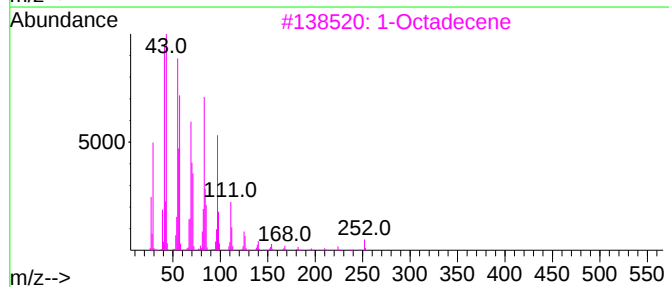
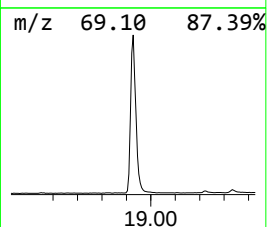
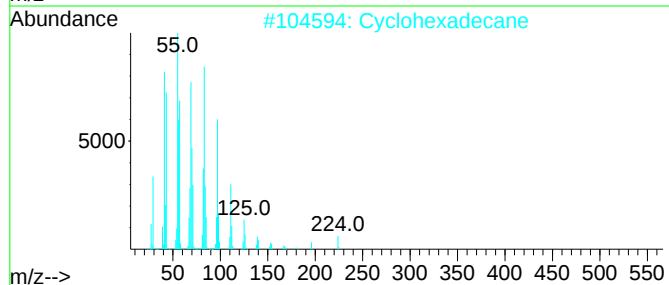
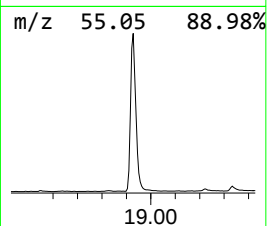
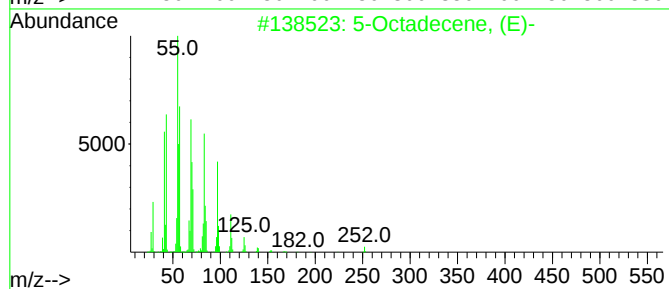
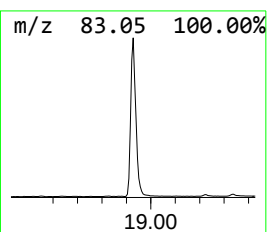
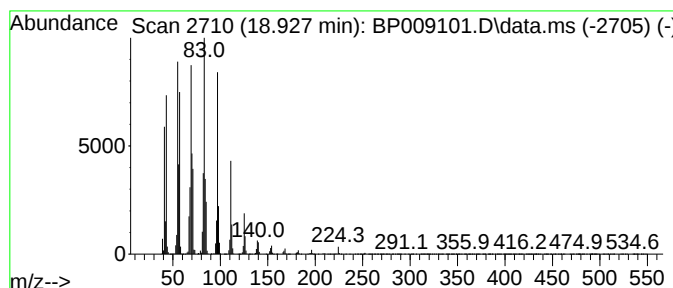
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.927	68.15 ng	9488260	Phenanthrene-d10	17.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	99
2	Cyclohexadecane	224	C16H32	000295-65-8	98
3	1-Octadecene	252	C18H36	000112-88-9	98
4	Cetene	224	C16H32	000629-73-2	96
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021022\
Data File : BP009101.D
Acq On : 10 Feb 2022 16:08
Operator : CG/JU
Sample : N1435-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-369

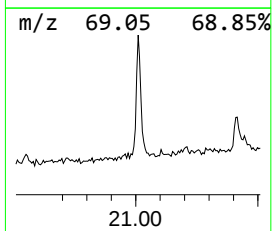
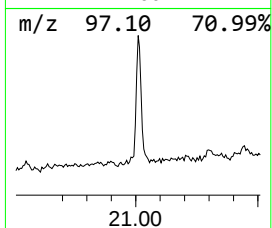
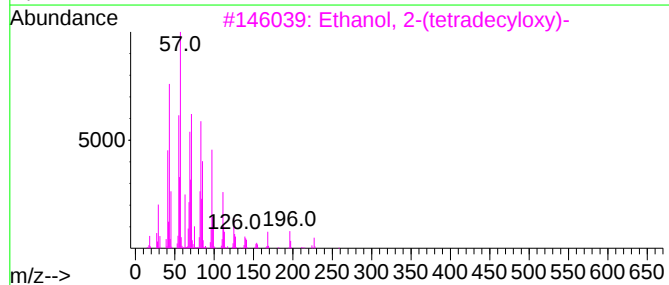
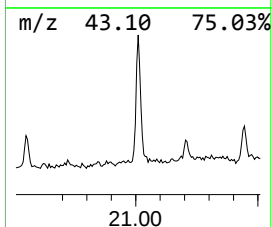
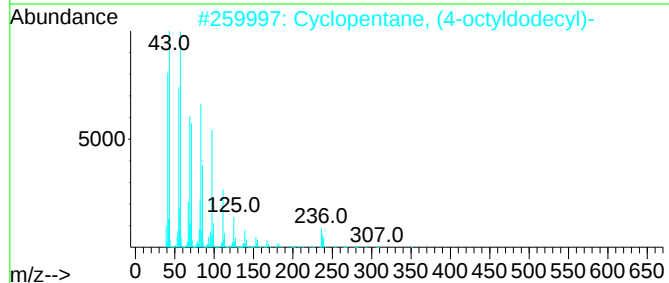
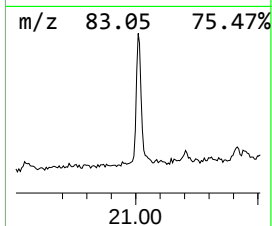
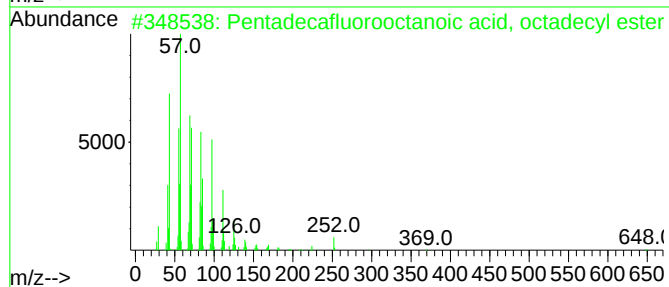
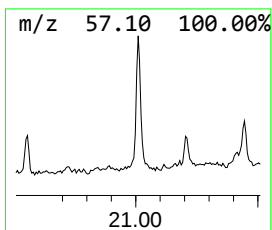
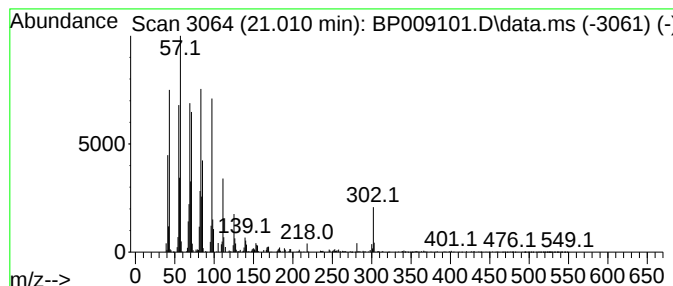
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	4.09 ng	854468	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	90
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021022\
Data File : BP009101.D
Acq On : 10 Feb 2022 16:08
Operator : CG/JU
Sample : N1435-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-369

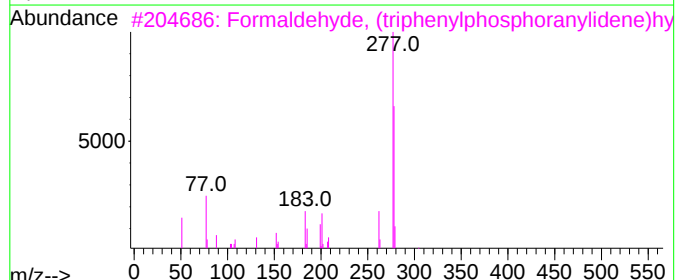
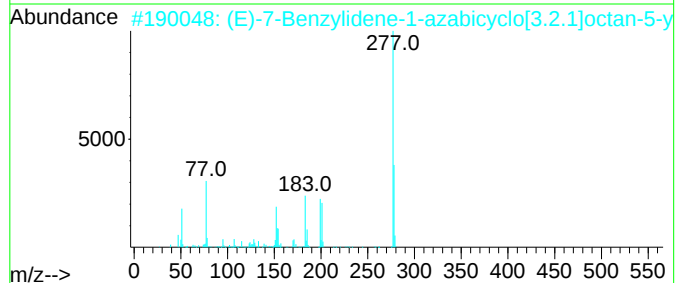
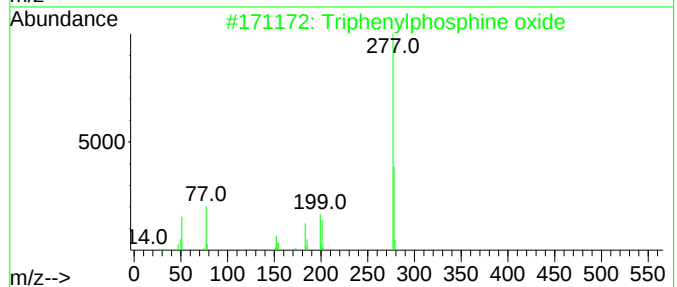
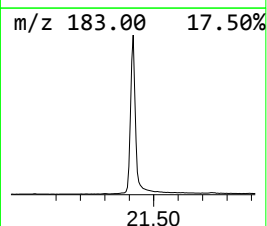
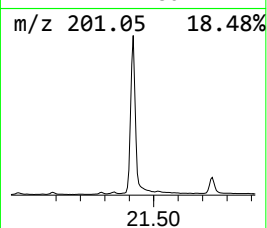
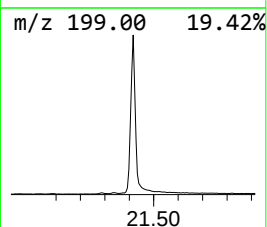
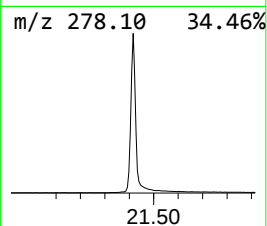
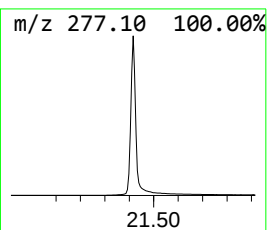
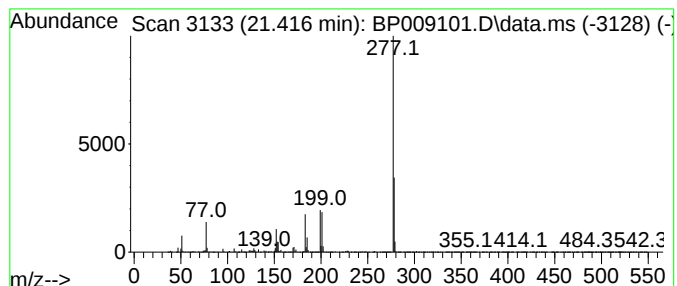
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	56.88 ng	11884400	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	47
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021022\
Data File : BP009101.D
Acq On : 10 Feb 2022 16:08
Operator : CG/JU
Sample : N1435-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-369

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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
Butane, 2-metho...	3.011	5.8	ng	338813	1	7.805	1158350	20.0
Propylene Glycol	3.558	18.5	ng	1069380	1	7.805	1158350	20.0
Phenanthrene, 1...	18.075	2.4	ng	326581	4	17.204	2784440	20.0
n-Hexadecanoic ...	18.104	7.7	ng	1076070	4	17.204	2784440	20.0
4H-Cyclopenta[d...	18.263	4.2	ng	590758	4	17.204	2784440	20.0
5-Octadecene, (E)-	18.927	68.2	ng	9488260	4	17.204	2784440	20.0
Pentadecafluoro...	21.010	4.1	ng	854468	5	21.298	4178860	20.0
Triphenylphosph...	21.416	56.9	ng	11884400	5	21.298	4178860	20.0