

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
 Data File : BP003340.D
 Acq On : 22 Sep 2020 15:47
 Operator : CG/JU
 Sample : L4099-08
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 105

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\8270-BP091520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003340.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.187	383	391	407	rBV	1874424	2981752	59.61%	7.420%
2	6.769	652	660	686	rBV	1882839	3123779	62.45%	7.773%
3	7.181	725	730	745	rBV	61273	118816	2.38%	0.296%
4	7.569	789	796	805	rVB	545555	834588	16.68%	2.077%
5	8.722	983	992	1015	rBV	1241077	2172575	43.43%	5.406%
6	10.346	1259	1268	1286	rBV	677155	1212121	24.23%	3.016%
7	12.834	1684	1691	1715	rBV	2570269	4039361	80.75%	10.051%
8	13.134	1736	1742	1762	rVB	525965	846727	16.93%	2.107%
9	13.681	1828	1835	1847	rBV	444348	662315	13.24%	1.648%
10	14.222	1919	1927	1935	rBV	1087524	1675111	33.49%	4.168%
11	15.369	2117	2122	2138	rBV	107167	172919	3.46%	0.430%
12	15.716	2174	2181	2205	rBV	2442927	3809727	76.16%	9.480%
13	16.975	2388	2395	2399	rBV	1403159	1997071	39.92%	4.969%
14	17.016	2399	2402	2408	rVV	111055	159509	3.19%	0.397%
15	17.110	2409	2418	2424	rVB2	27723	54458	1.09%	0.136%
16	17.386	2457	2465	2475	rBV3	22307	50228	1.00%	0.125%
17	17.898	2548	2552	2558	rBV2	46008	66980	1.34%	0.167%
18	18.039	2570	2576	2580	rBV2	37291	65132	1.30%	0.162%
19	18.722	2688	2692	2700	rBV2	92884	173598	3.47%	0.432%
20	18.998	2734	2739	2743	rBV	401525	523579	10.47%	1.303%
21	19.033	2743	2745	2749	rVB	72725	70402	1.41%	0.175%
22	19.345	2790	2798	2808	rBV	387816	633897	12.67%	1.577%
23	19.551	2826	2833	2838	rBV	4137986	5002406	100.00%	12.448%
24	19.669	2848	2853	2859	rBV4	31461	73243	1.46%	0.182%
25	19.833	2878	2881	2885	rVB2	79003	99233	1.98%	0.247%
26	19.933	2894	2898	2901	rBV	48602	59467	1.19%	0.148%
27	20.798	3041	3045	3052	rBV	897917	1162597	23.24%	2.893%
28	21.068	3084	3091	3095	rBV	2111973	2898176	57.94%	7.212%
29	21.104	3095	3097	3107	rVB	271570	316719	6.33%	0.788%
30	21.233	3114	3119	3124	rBV2	62342	117070	2.34%	0.291%
31	21.657	3188	3191	3200	rBV5	88022	183639	3.67%	0.457%
32	22.110	3263	3268	3273	rVB2	105424	166937	3.34%	0.415%
33	22.604	3347	3352	3357	rBV	341367	689192	13.78%	1.715%
34	23.068	3427	3431	3440	rVB	134485	253092	5.06%	0.630%
35	23.168	3442	3448	3455	rBV	325111	575904	11.51%	1.433%
36	23.263	3457	3464	3470	rBV	1398524	2550040	50.98%	6.345%

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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\8270-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.810	3552	3557	3564	rVB	144613	274626	5.49%	0.683%
38	23.892	3566	3571	3583	rVB4	135176	320535	6.41%	0.798%

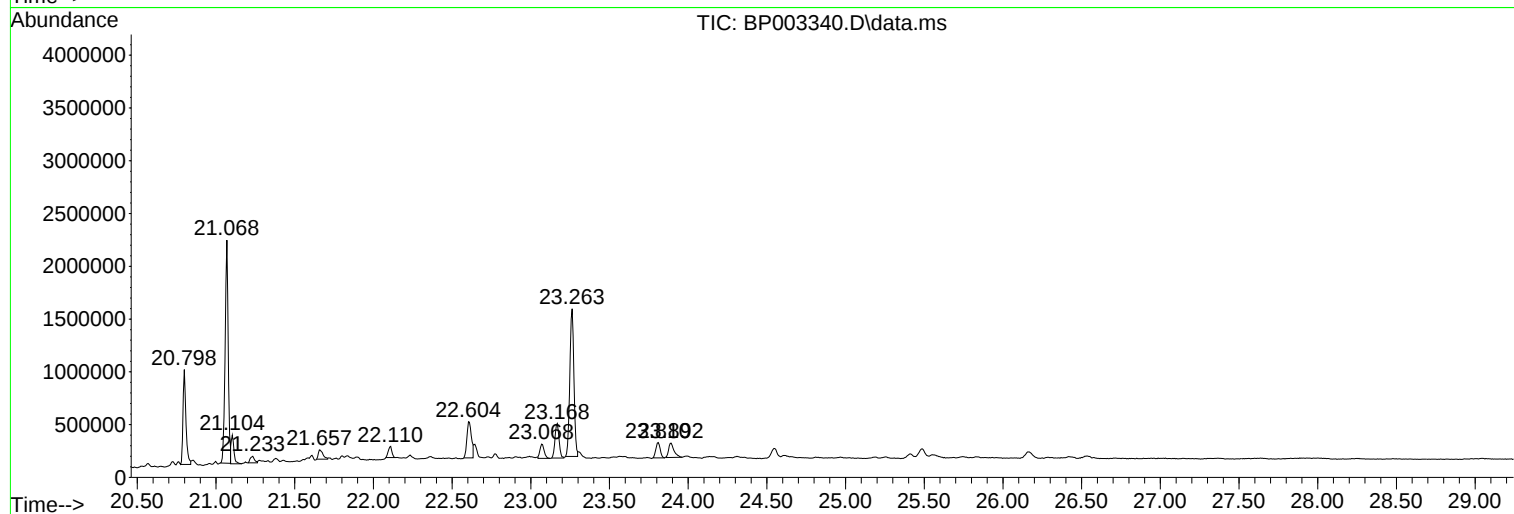
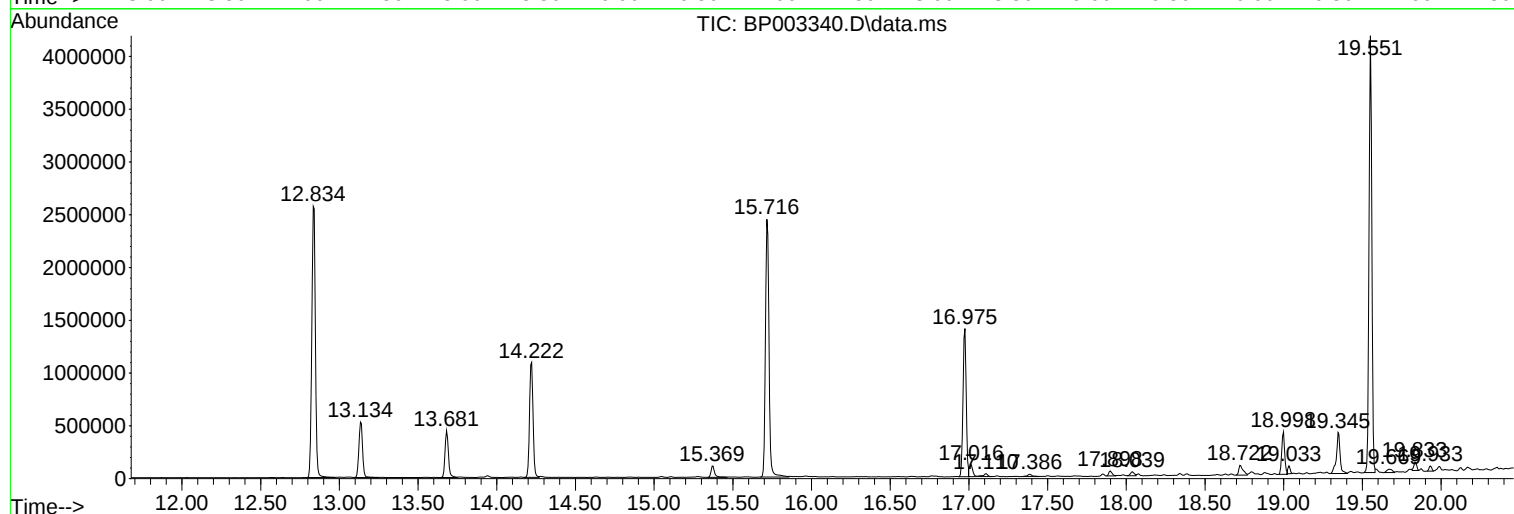
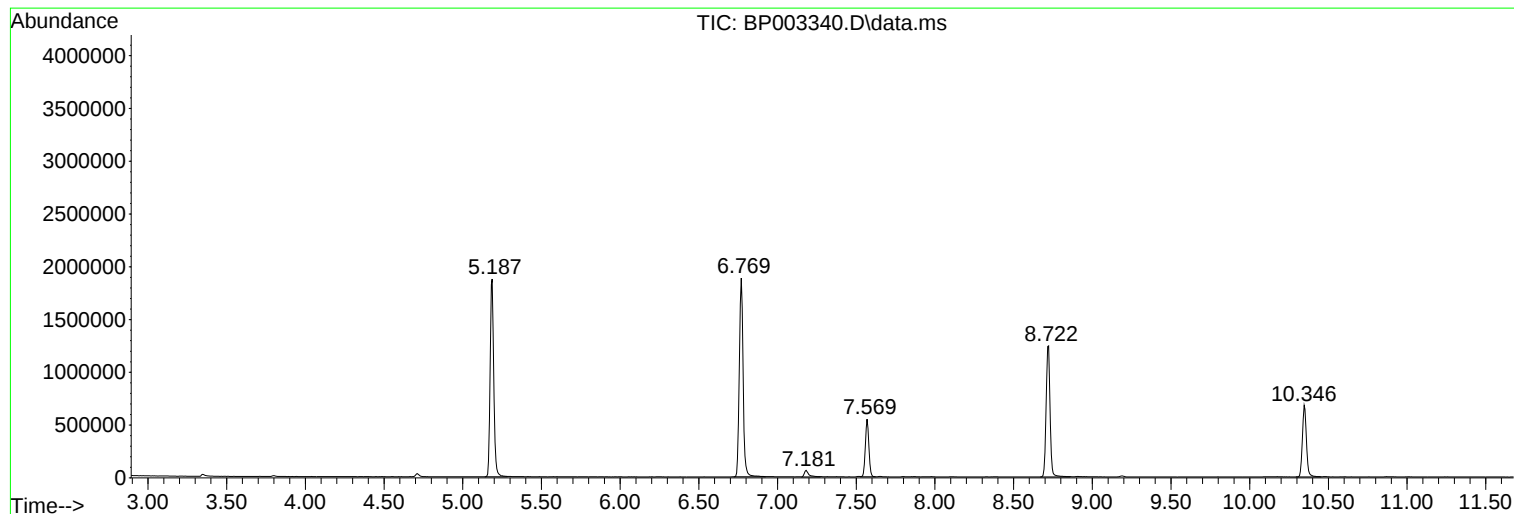
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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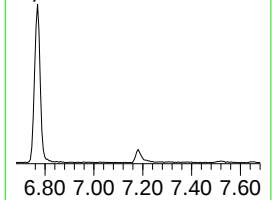
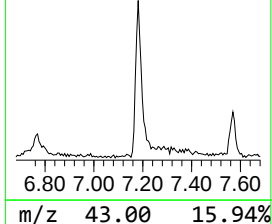
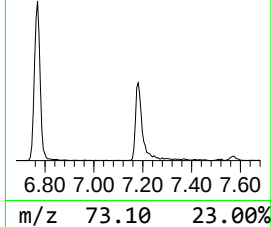
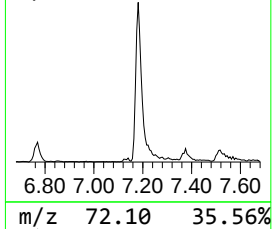
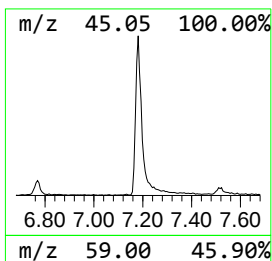
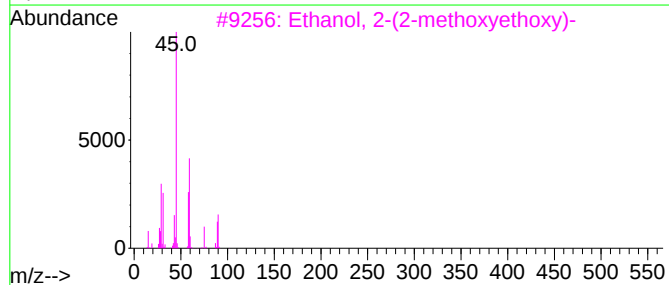
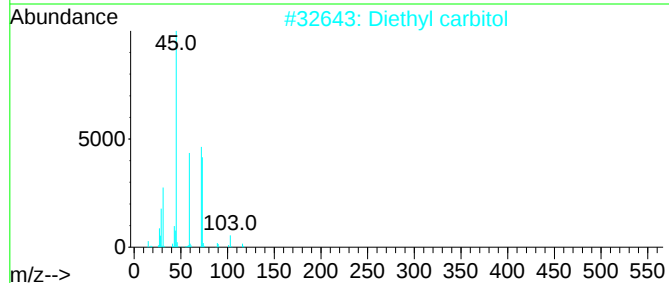
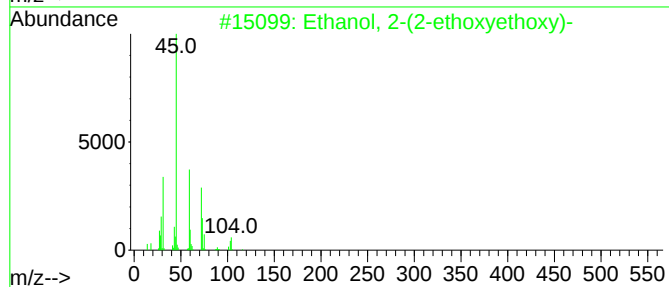
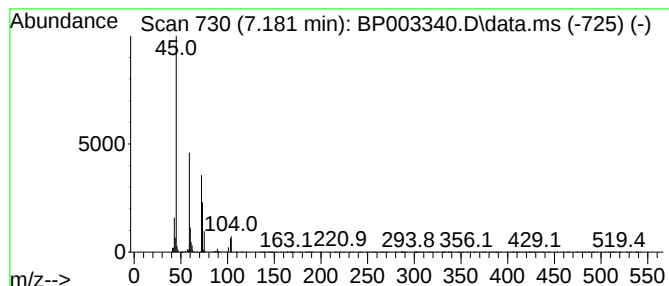
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	2.85 ng	118816	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	86
2			Diethyl carbitol	162	C8H18O3	000112-36-7	64
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	53
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
5			Acetic acid, (2-ethoxy)ethoxy-, ...	162	C7H14O4	016326-34-4	39



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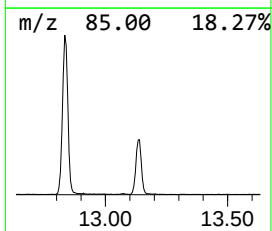
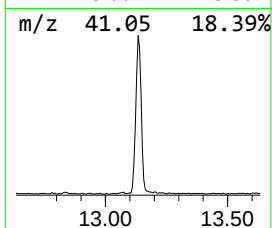
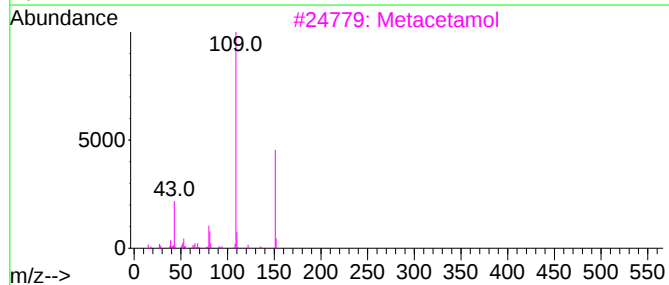
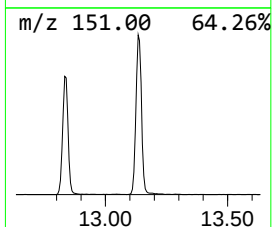
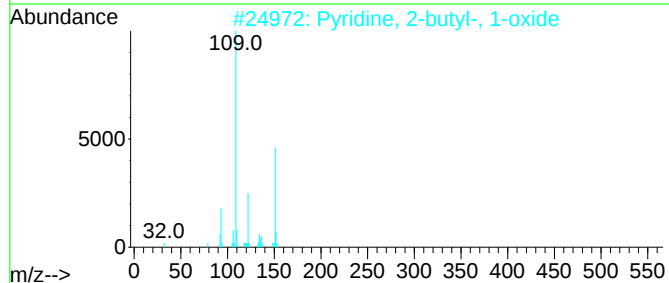
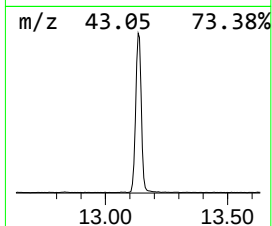
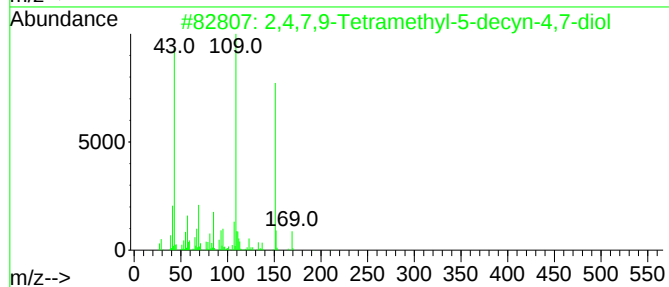
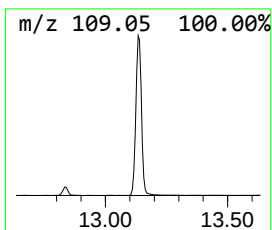
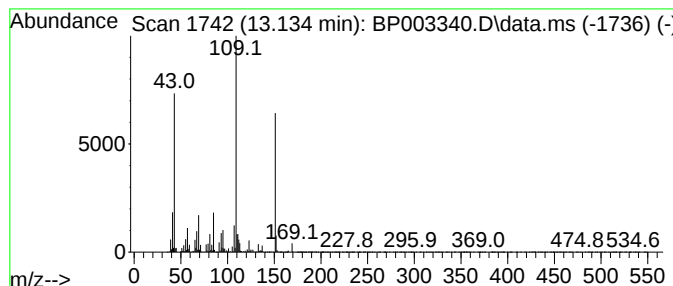
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.134	10.11 ng	846727	Acenaphthene-d10		14.222	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	Metacetamol		151	C8H9NO2	000621-42-1	53
4	m-Isopropoxyaniline		151	C9H13NO	041406-00-2	53
5	2-Propenal, 3-(2,2,6-trimethyl-7...		194	C12H18O2	055759-91-6	50



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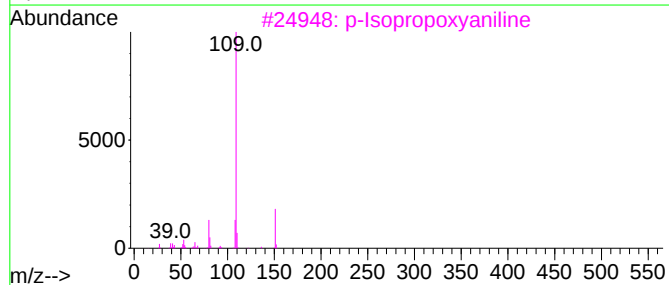
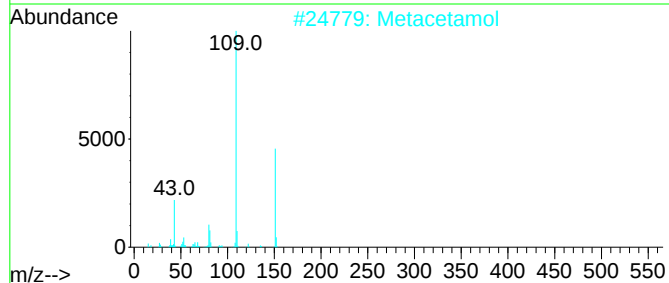
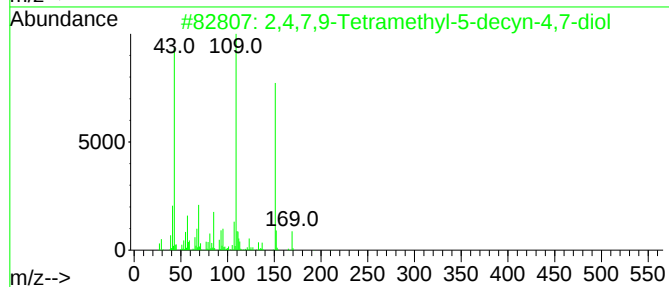
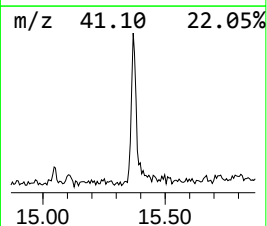
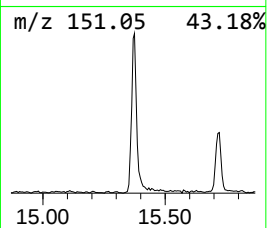
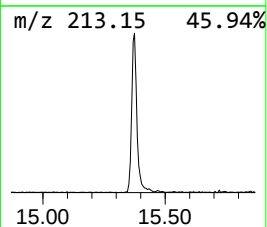
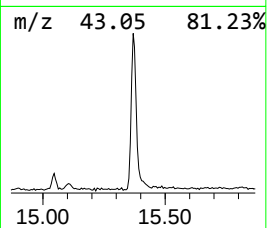
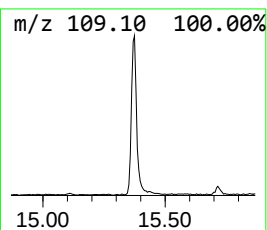
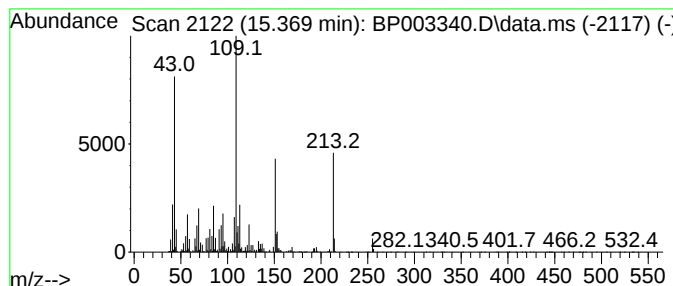
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.36 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.369	2.06 ng	172919	Acenaphthene-d10	14.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53		
2	Metacetamol	151	C8H9NO2	000621-42-1	43		
3	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	38		
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	38		
5	1,2-Diazaspiro[4.4]nonen-3-carbo...	238	C13H22N2O2	1000164-25-8	30		



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ClientSampleId :
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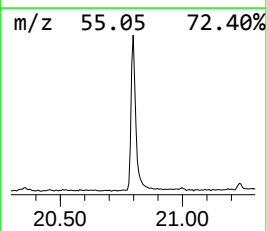
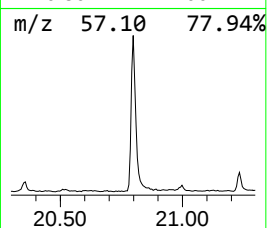
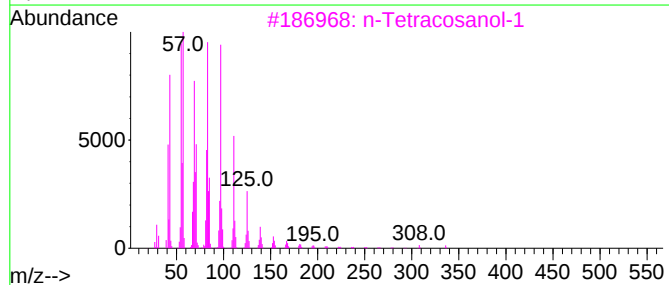
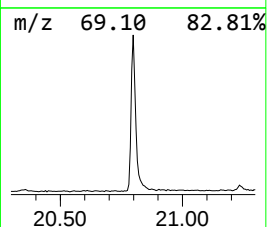
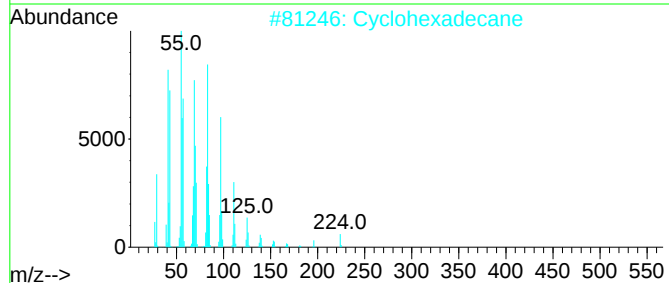
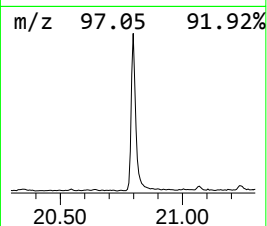
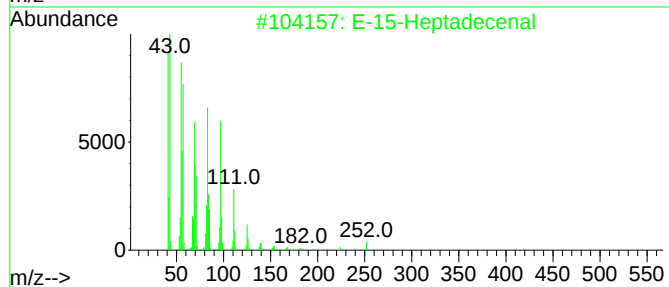
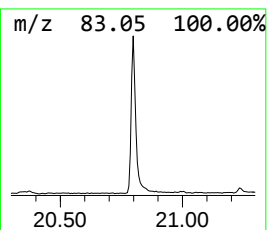
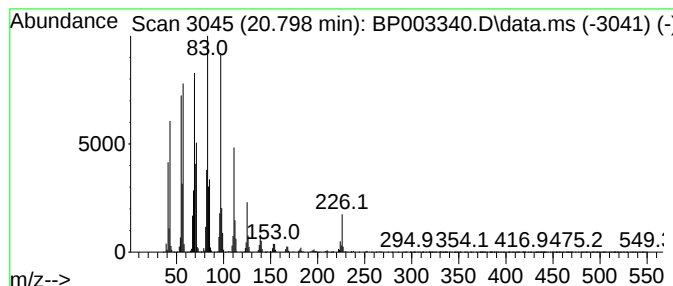
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 E-15-Heptadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.798	8.02 ng	1162600	Chrysene-d12	21.069

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		E-15-Heptadecenal	252	C17H32O	1000130-97-9	98
2		Cyclohexadecane	224	C16H32	000295-65-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Behenic alcohol	326	C22H46O	000661-19-8	94
5		Cyclopentadecane	210	C15H30	000295-48-7	93



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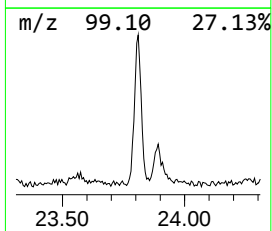
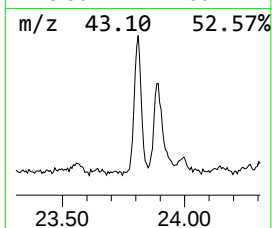
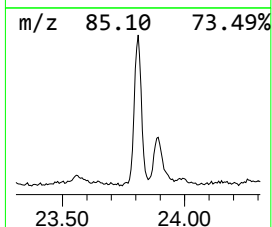
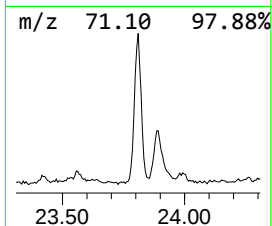
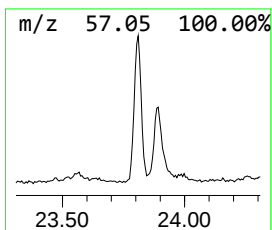
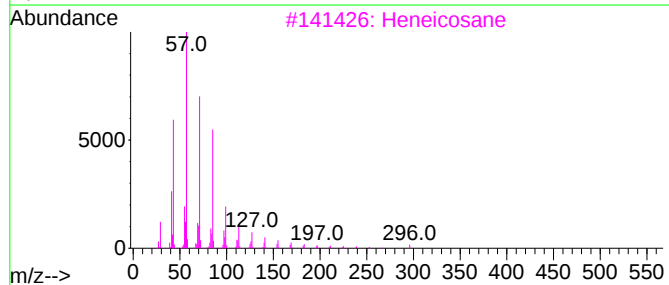
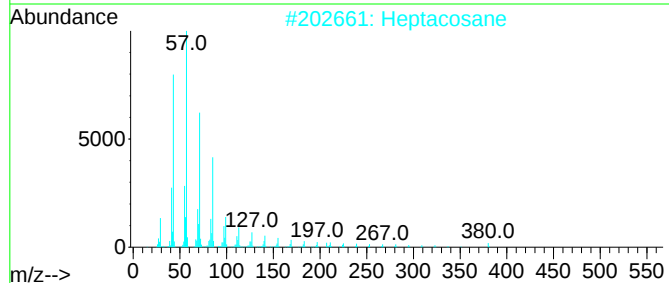
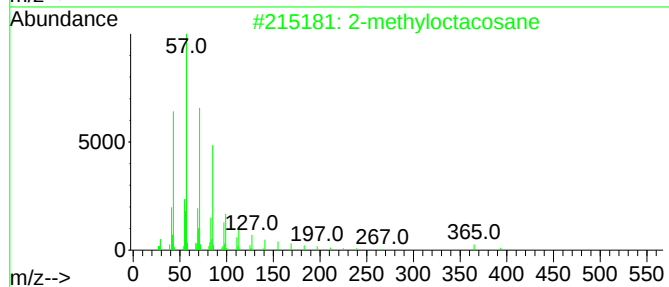
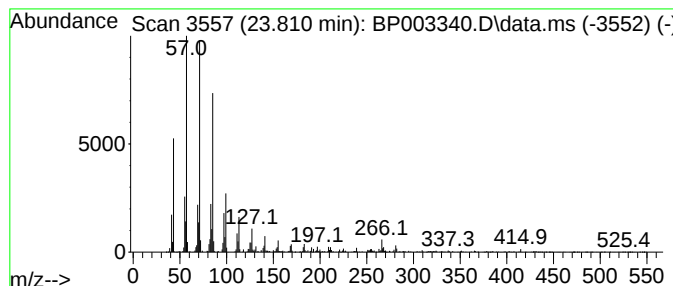
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.810	2.15 ng	274626	Perylene-d12	23.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Heptacosane	380	C27H56	000593-49-7	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
5			Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003340.D
Acq On : 22 Sep 2020 15:47
Operator : CG/JU
Sample : L4099-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
105

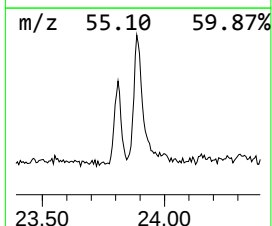
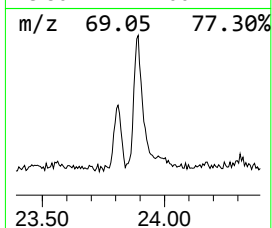
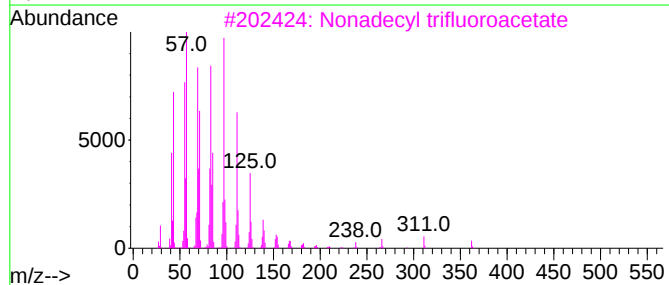
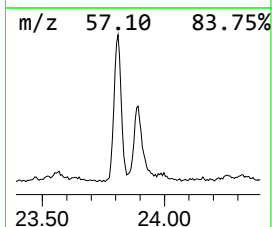
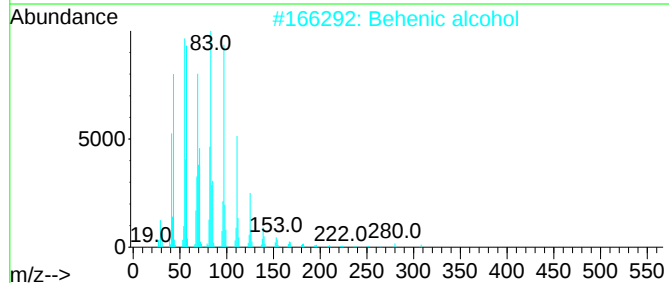
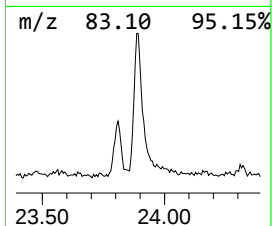
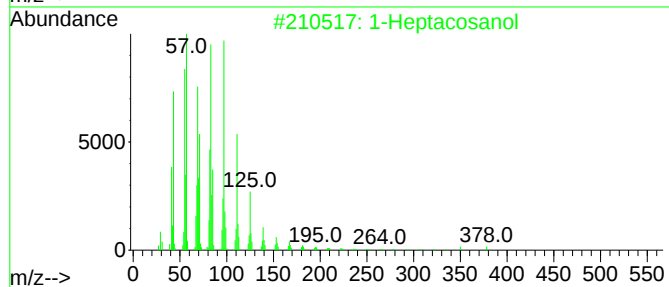
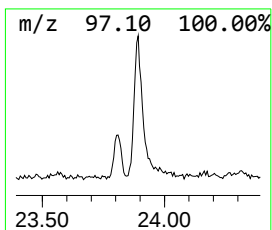
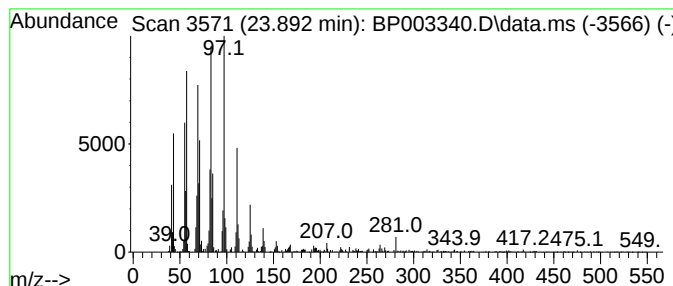
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.892	2.51 ng	320535	Perylene-d12	23.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	89
4			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	87
5			1-Nonadecene	266	C19H38	018435-45-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092220\
Data File : BP003340.D
Acq On : 22 Sep 2020 15:47
Operator : CG/JU
Sample : L4099-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
105

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-e...	7.181	2.9	ng	118816	1	7.569	834588	20.0
2,4,7,9-Tetrame...	13.134	10.1	ng	846727	3	14.222	1675110	20.0
unknown15.36	15.369	2.1	ng	172919	3	14.222	1675110	20.0
E-15-Heptadecenal	20.798	8.0	ng	1162600	5	21.069	2898180	20.0
2-methyloctacosane	23.810	2.1	ng	274626	6	23.262	2550040	20.0
1-Heptacosanol	23.892	2.5	ng	320535	6	23.262	2550040	20.0