

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
 Data File : BP003979.D
 Acq On : 17 Nov 2020 17:20
 Operator : CG/JU
 Sample : L4770-21
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FJ-BH-04-2-3

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-BP110320.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.923	3	6	19	rVB	4195259	5096774	97.22%	15.018%
2	3.081	27	33	43	rVV	110087	200671	3.83%	0.591%
3	3.175	44	49	61	rVB	329519	440369	8.40%	1.298%
4	5.275	398	406	413	rVB	97358	140419	2.68%	0.414%
5	5.805	488	496	509	rBV	1689153	2537298	48.40%	7.477%
6	7.452	767	776	790	rBV	1720706	2768594	52.81%	8.158%
7	8.281	909	917	924	rBV	470869	760057	14.50%	2.240%
8	9.440	1106	1114	1127	rBV	1079279	1807576	34.48%	5.326%
9	11.110	1390	1398	1407	rBV	621404	1038650	19.81%	3.061%
10	13.522	1800	1808	1832	rBV	2408254	3682675	70.25%	10.852%
11	13.787	1849	1853	1860	rVB	54711	80963	1.54%	0.239%
12	14.328	1937	1945	1954	rBV	372292	539966	10.30%	1.591%
13	14.904	2036	2043	2058	rBV	908652	1372753	26.19%	4.045%
14	16.387	2288	2295	2312	rBV	1623002	2456069	46.85%	7.237%
15	17.633	2501	2507	2517	rBV	1128757	1634198	31.17%	4.815%
16	19.228	2773	2778	2785	rBV	155139	185654	3.54%	0.547%
17	20.133	2927	2932	2939	rBV	4433359	5242436	100.00%	15.448%
18	21.322	3130	3134	3143	rBV	377231	486362	9.28%	1.433%
19	21.669	3188	3193	3207	rVB	1326327	1859466	35.47%	5.479%
20	24.157	3609	3616	3624	rBV	791874	1605765	30.63%	4.732%

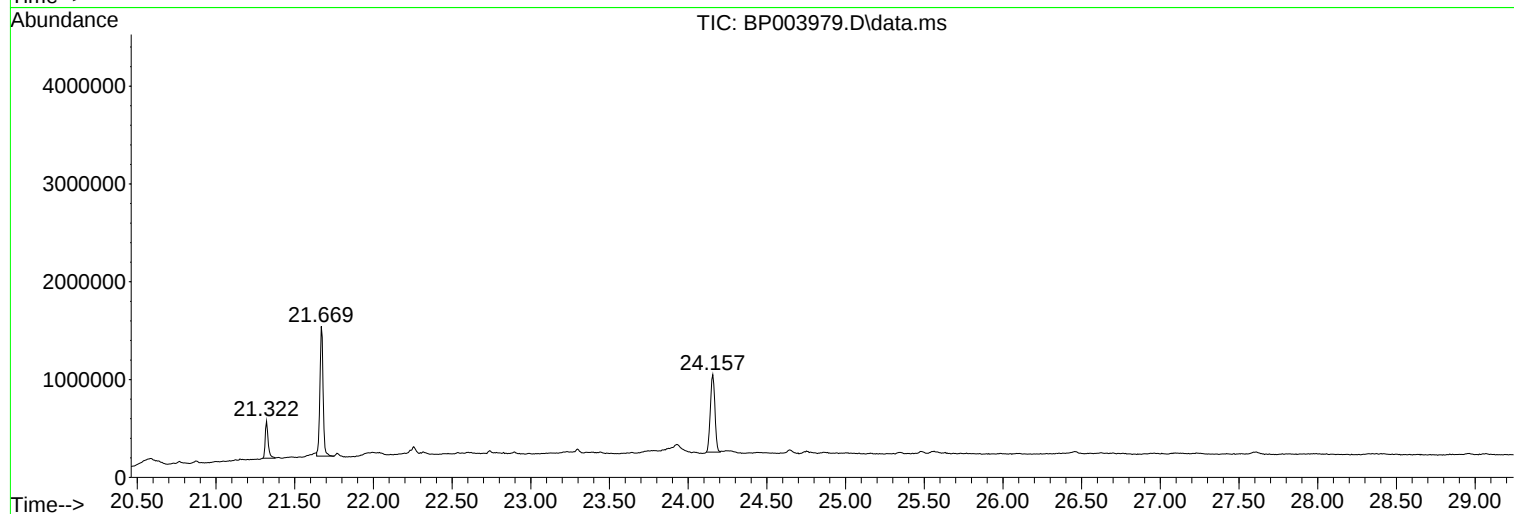
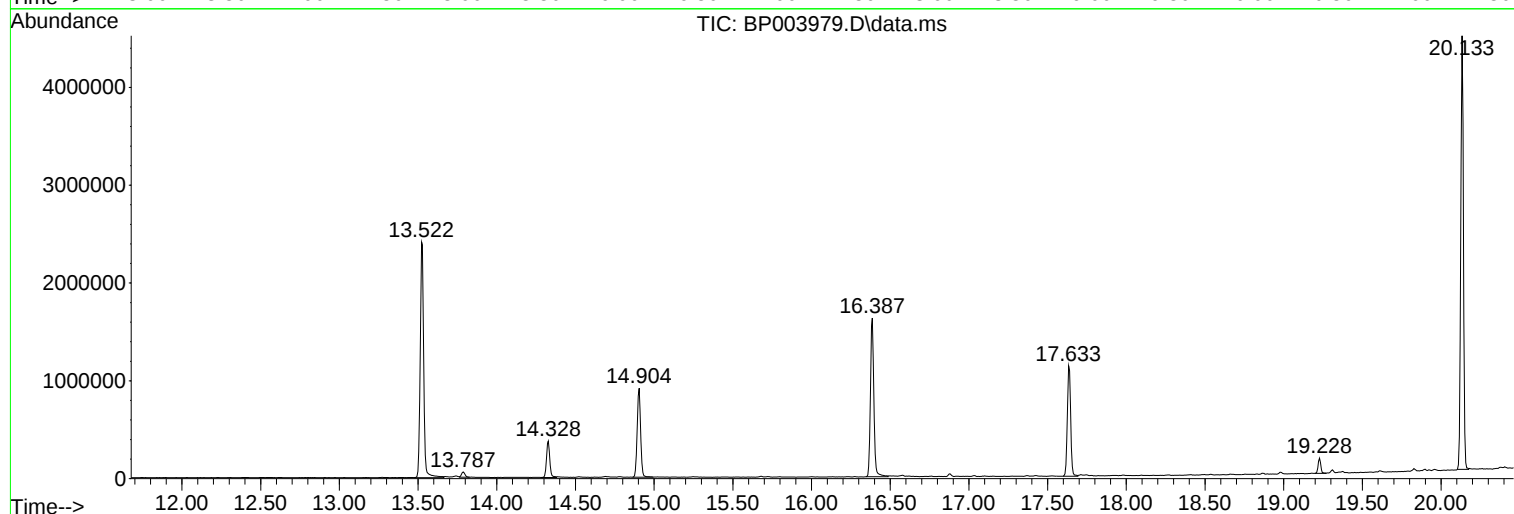
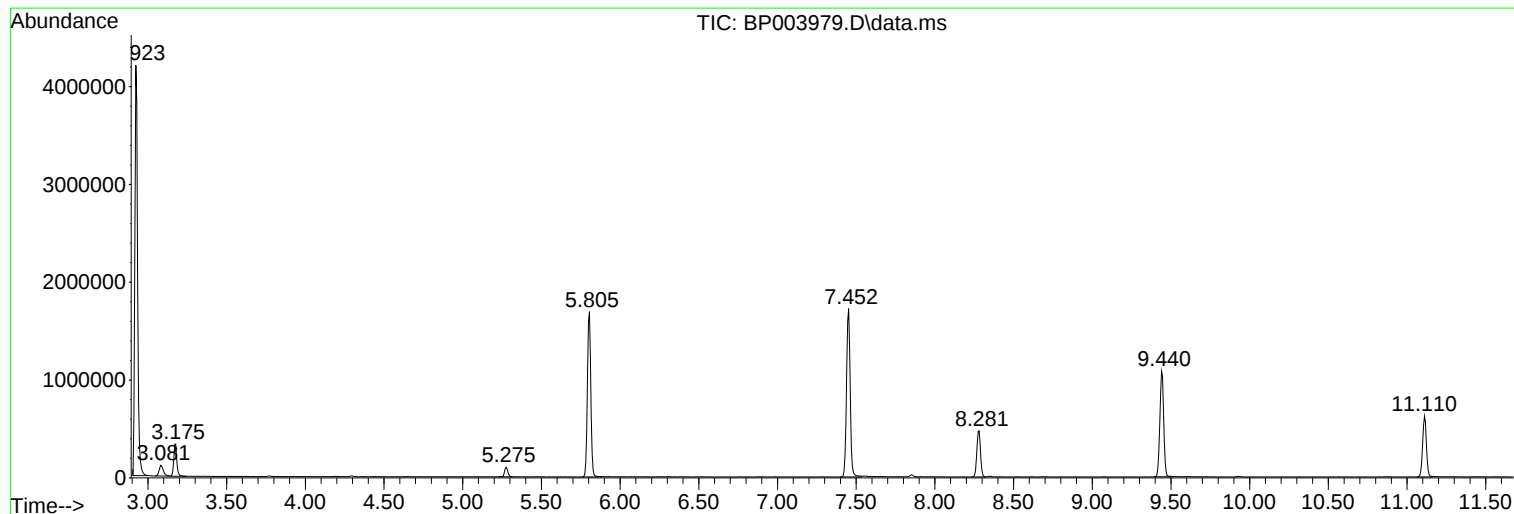
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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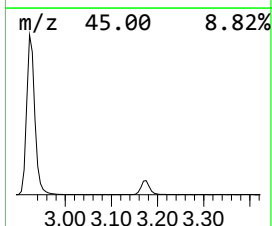
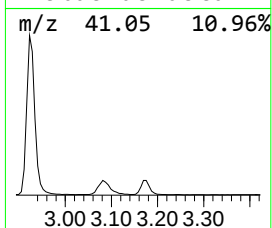
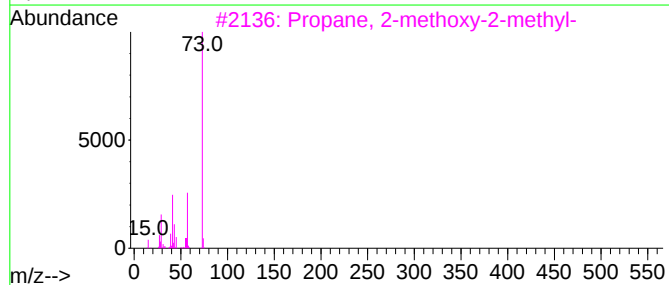
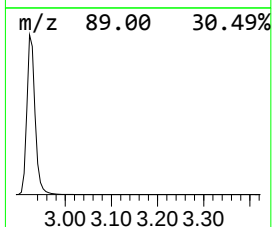
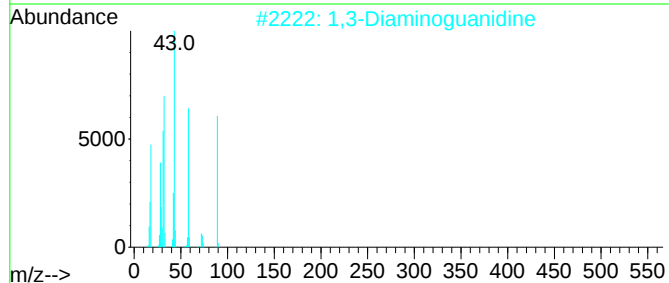
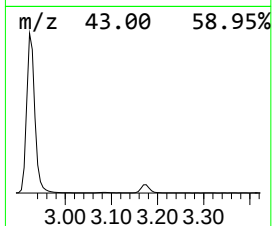
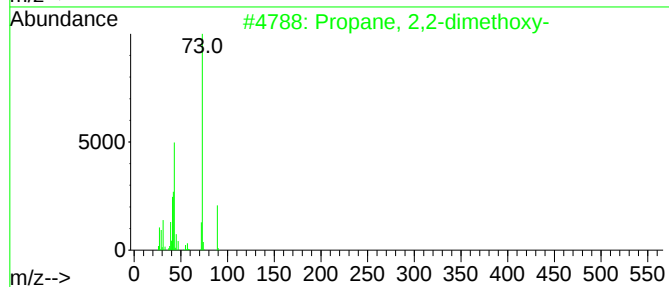
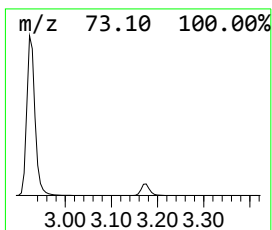
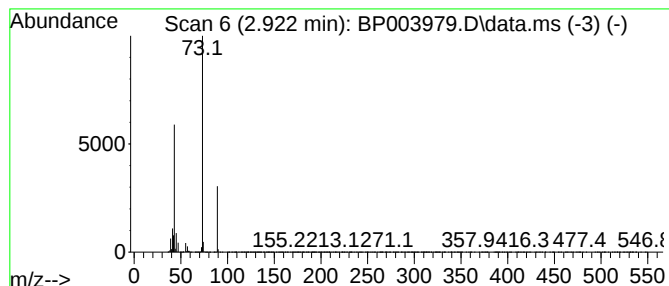
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	134.12 ng	5096770	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9



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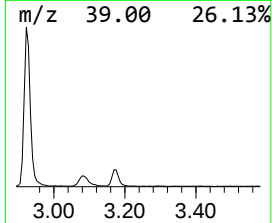
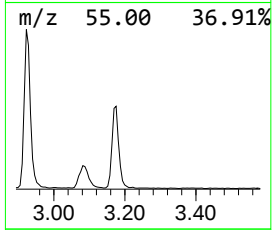
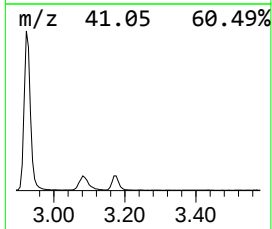
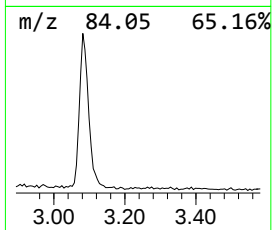
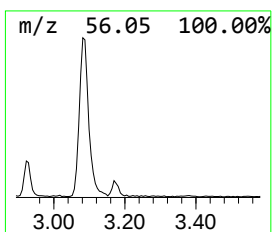
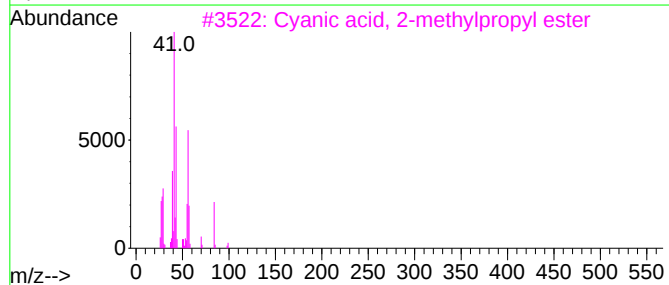
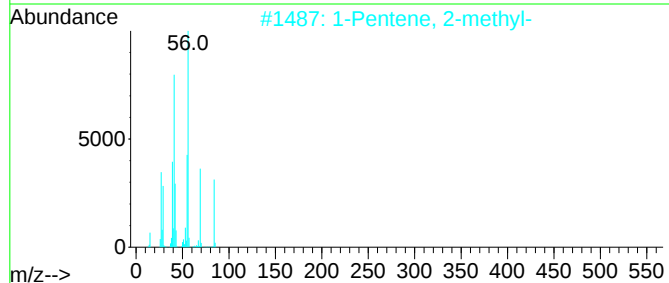
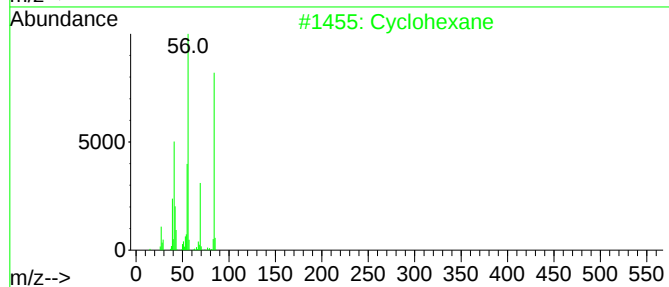
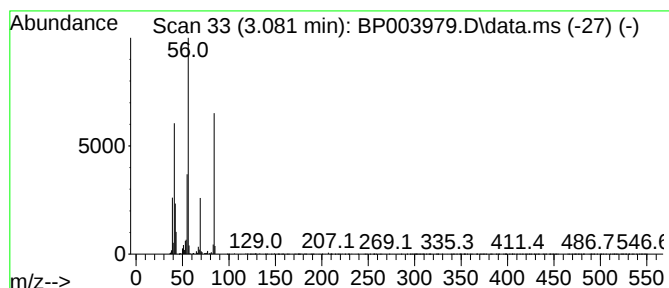
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	5.28 ng	200671	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	94
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3			Cyanoic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
4			1-Hexene	84	C6H12	000592-41-6	53
5			Vigabatrin	129	C6H11NO2	060643-86-9	50



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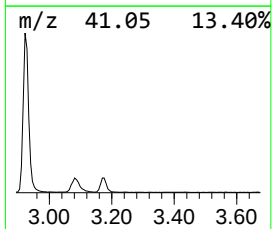
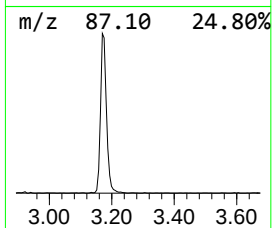
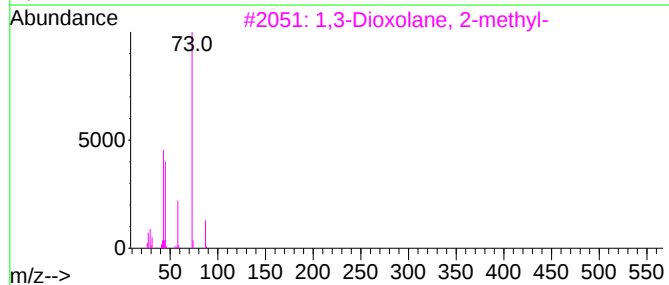
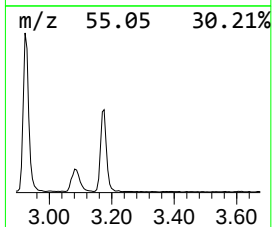
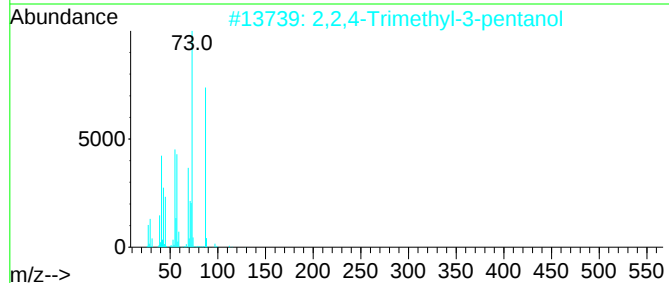
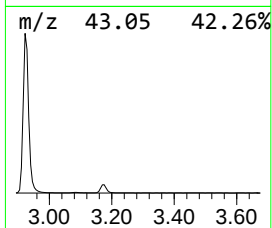
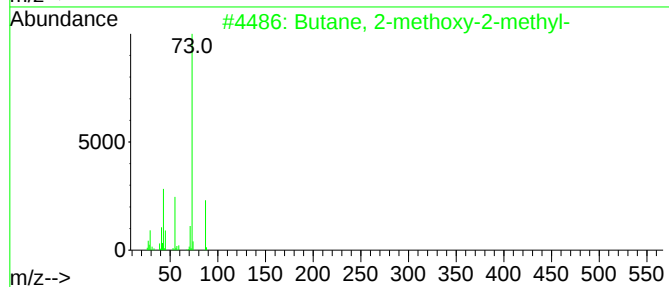
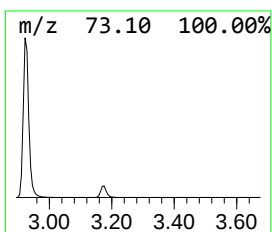
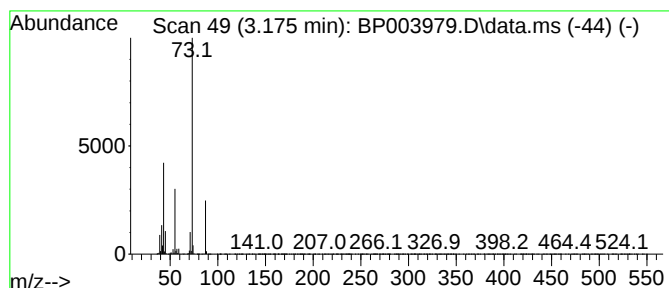
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	11.59 ng	440369	1,4-Dichlorobenzene-d4	8.281

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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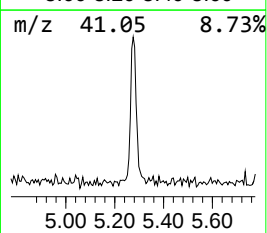
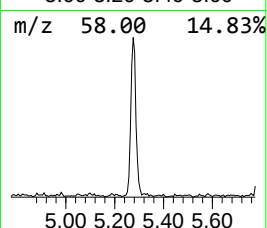
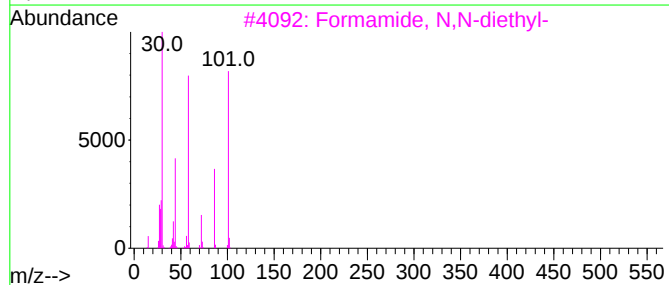
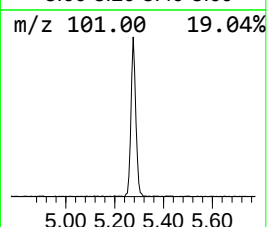
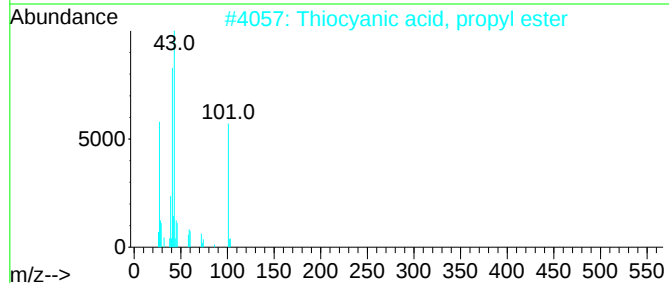
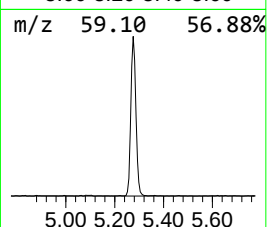
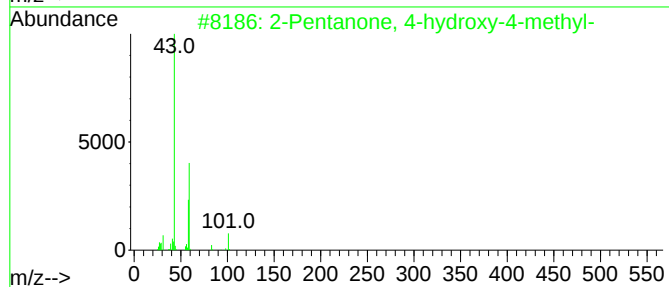
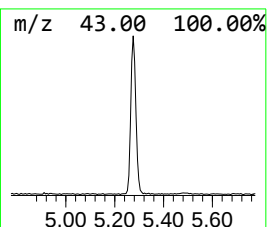
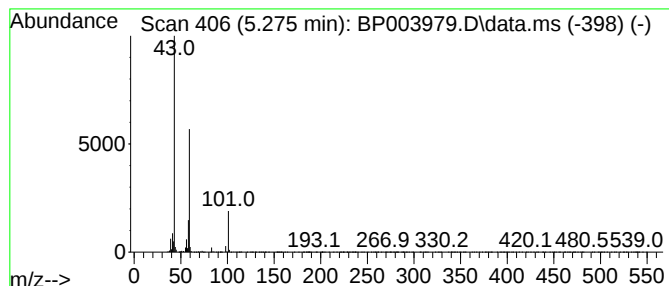
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.275	3.69 ng	140419	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
2			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
3			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4			Hexanamide	115	C6H13NO	000628-02-4	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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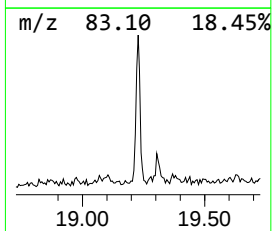
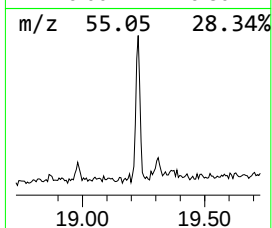
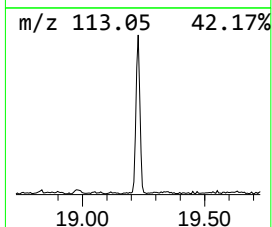
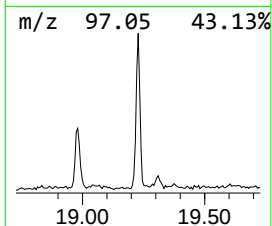
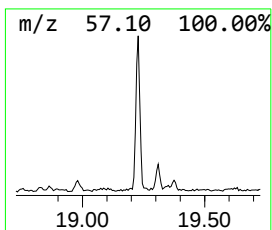
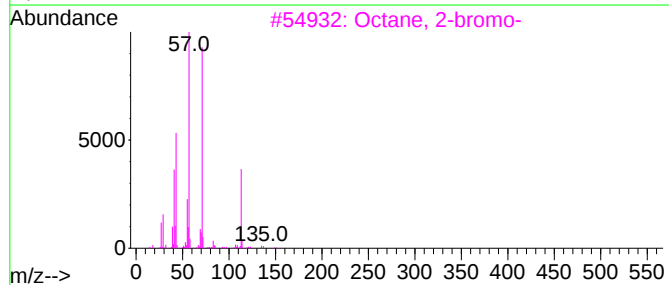
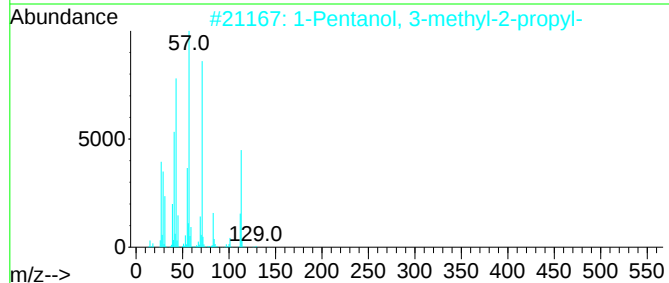
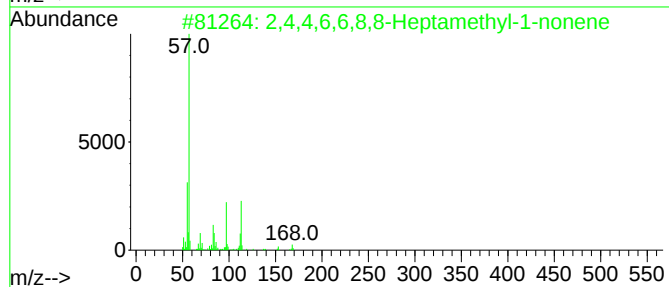
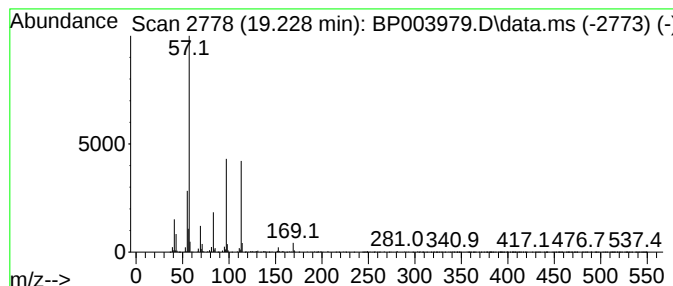
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Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	2.27 ng	185654	Phenanthrene-d10	17.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	72		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40		
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38		
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	35		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	32		



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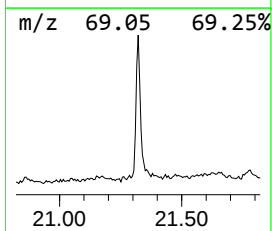
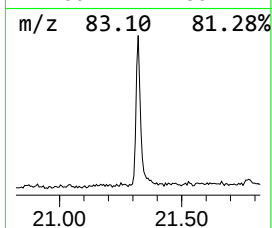
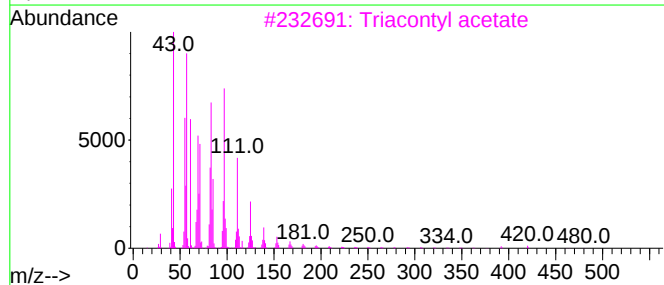
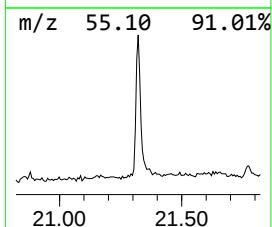
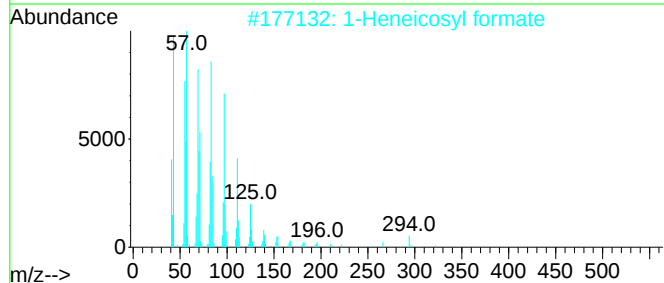
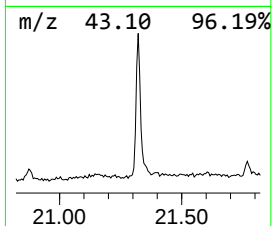
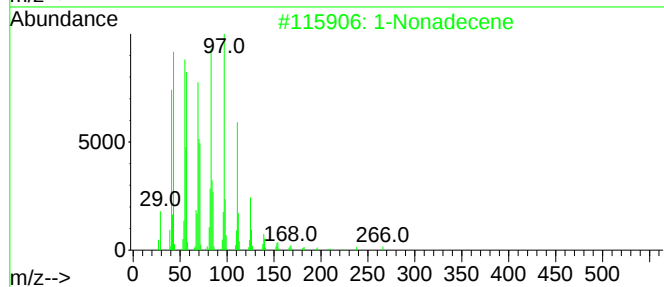
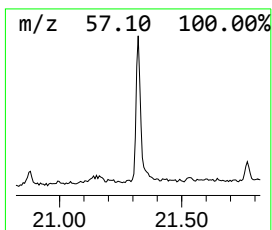
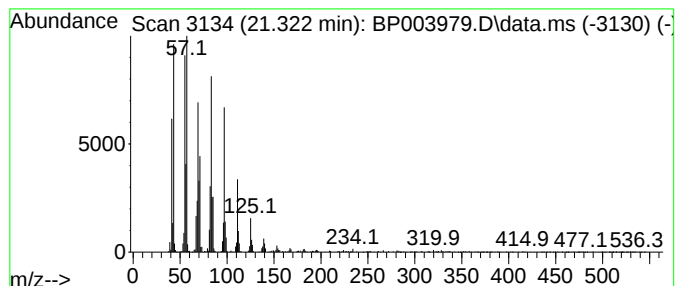
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.322	5.23 ng	486362	Chrysene-d12	21.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	97
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
3			Triacontyl acetate	480	C32H64O2	041755-58-2	95
4			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
Data File : BP003979.D
Acq On : 17 Nov 2020 17:20
Operator : CG/JU
Sample : L4770-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FJ-BH-04-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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
Propane, 2,2-di...	2.922	134.1	ng	5096770	1	8.281	760057	20.0
Cyclohexane	3.081	5.3	ng	200671	1	8.281	760057	20.0
Butane, 2-metho...	3.175	11.6	ng	440369	1	8.281	760057	20.0
2-Pentanone, 4-...	5.275	3.7	ng	140419	1	8.281	760057	20.0
2,4,4,6,6,8,8-H...	19.227	2.3	ng	185654	4	17.634	1634200	20.0
1-Nonadecene	21.322	5.2	ng	486362	5	21.669	1859470	20.0