

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
 Data File : BM033266.D
 Acq On : 26 Nov 2021 15:53
 Operator : CG/JU
 Sample : PB141003BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB141003BL

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_M\Methods\8270-BM112421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.455	186	190	200	rVB	73442	105439	1.82%	0.312%
2	5.055	287	292	301	rBV	719732	1010588	17.45%	2.994%
3	5.513	363	370	384	rBV	2759160	4020880	69.41%	11.911%
4	6.131	468	475	482	rBV	52054	84412	1.46%	0.250%
5	7.102	632	640	657	rBV	2550054	4159752	71.81%	12.322%
6	7.937	775	782	790	rBV	518615	834351	14.40%	2.472%
7	9.095	971	979	1001	rBV	1584748	2735462	47.22%	8.103%
8	10.731	1250	1257	1272	rVB	641839	1097251	18.94%	3.250%
9	13.183	1666	1674	1689	rBV	3480908	5215385	90.03%	15.449%
10	14.554	1900	1907	1917	rBV	849041	1285950	22.20%	3.809%
11	16.042	2153	2160	2176	rBV	2157071	3199737	55.24%	9.478%
12	17.295	2366	2373	2387	rVB	874585	1322137	22.82%	3.916%
13	19.901	2810	2816	2823	rBV	4762045	5792755	100.00%	17.159%
14	21.454	3075	3080	3085	rBV	1010685	1364523	23.56%	4.042%
15	23.783	3471	3476	3486	rVB2	761867	1529934	26.41%	4.532%

Sum of corrected areas: 33758556

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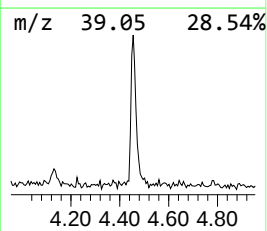
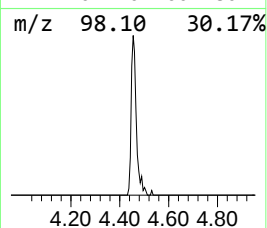
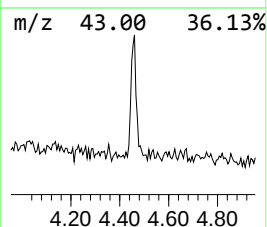
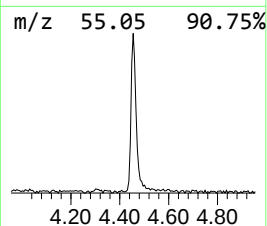
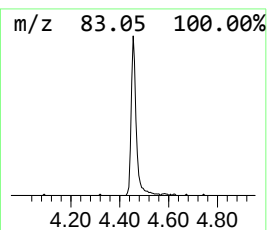
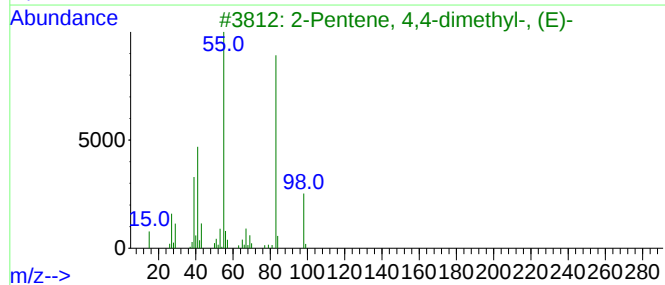
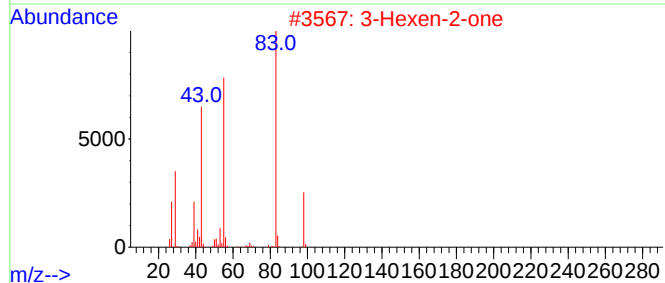
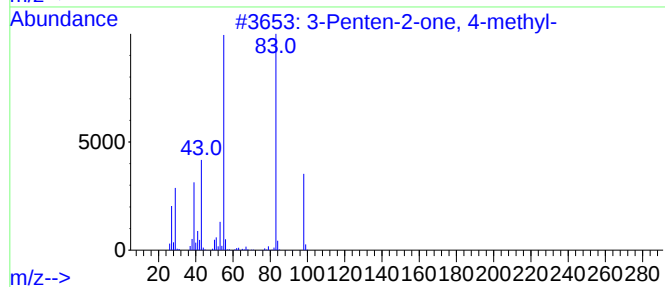
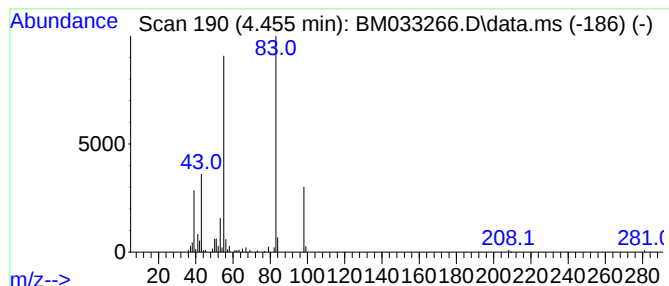
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.455	2.53 ng	105439	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	93
2	3-Hexen-2-one			98	C6H10O	000763-93-9	87
3	2-Pentene, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	86
4	2-Pentene, 2,4-dimethyl-			98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-			98	C7H14	026232-98-4	86



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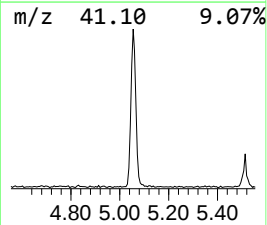
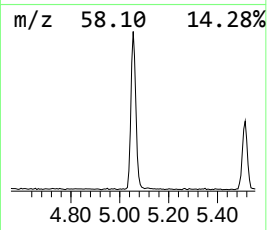
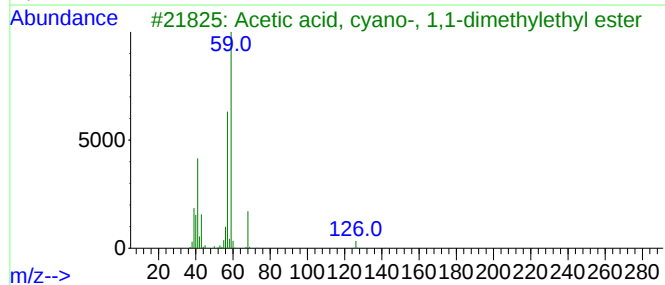
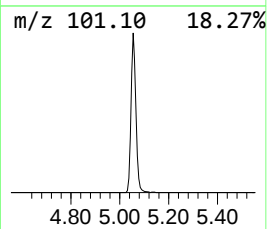
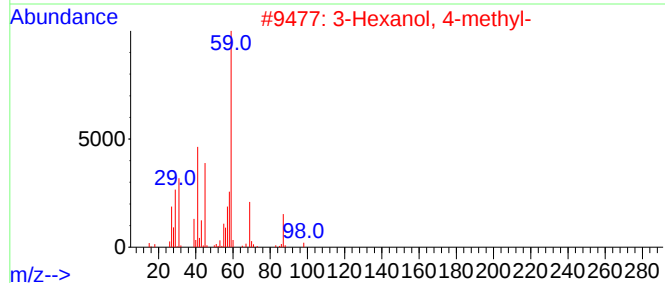
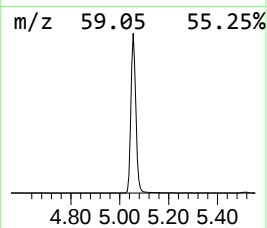
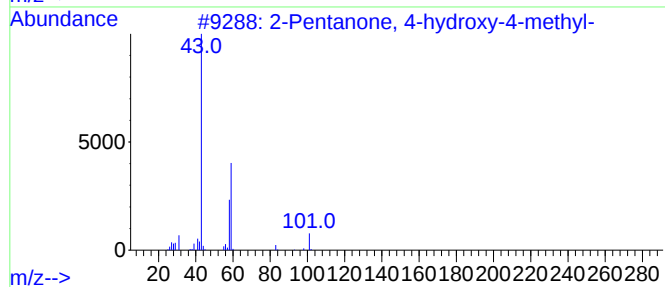
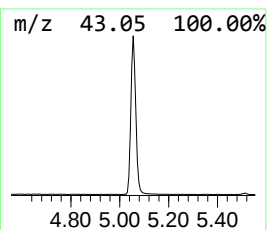
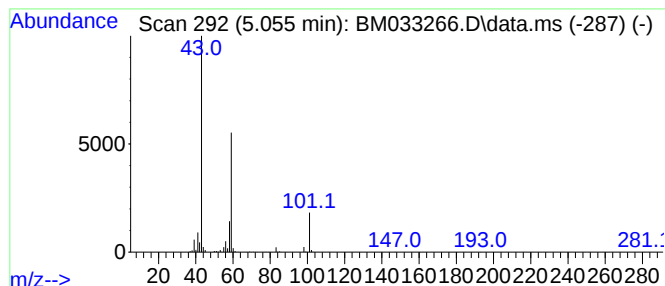
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.055	24.22 ng	1010590	1,4-Dichlorobenzene-d4	7.937	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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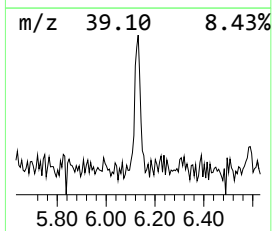
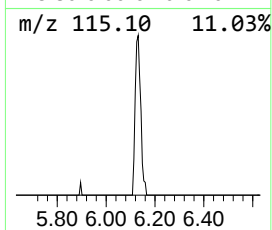
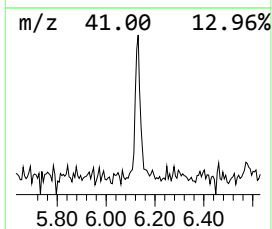
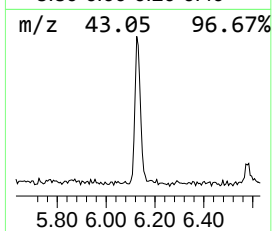
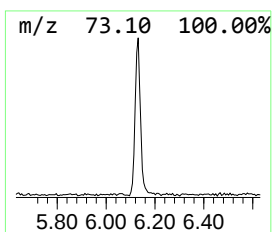
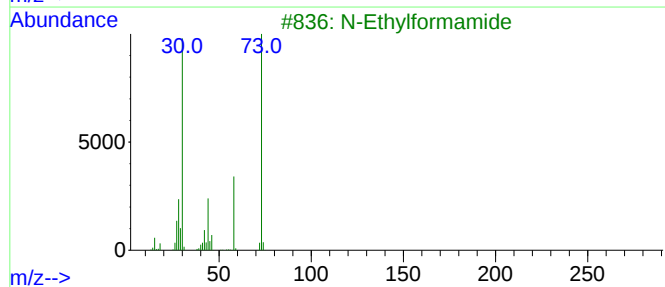
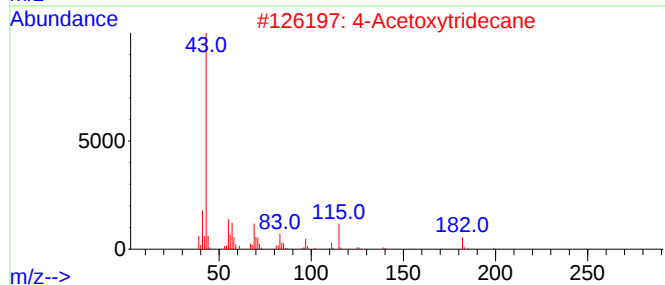
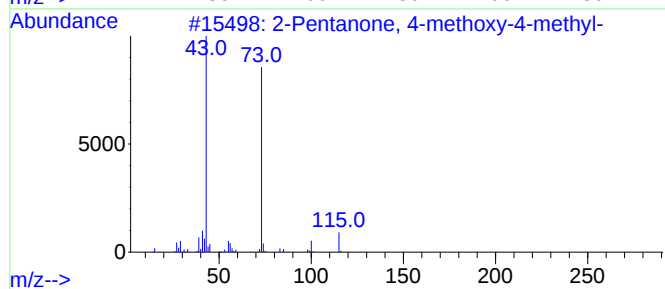
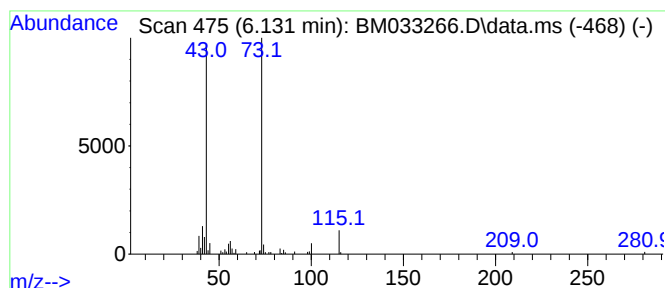
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
6.131	2.02 ng	84412	1,4-Dichlorobenzene-d4		7.937	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	78
2	4-Acetoxytridecane		242	C15H30O2	060826-30-4	23
3	N-Ethylformamide		73	C3H7NO	000627-45-2	16
4	3-Hexanol, 2-methyl-		116	C7H16O	000617-29-8	12
5	Pentane, 3-methoxy-		102	C6H14O	036839-67-5	12



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.455	2.5	ng	105439	1	7.937	834351	20.0
2-Pentanone, 4-...	5.055	24.2	ng	1010590	1	7.937	834351	20.0
2-Pentanone, 4-...	6.131	2.0	ng	84412	1	7.937	834351	20.0